Supplementary Material 1. Spatial Scaling Challenge Scene information provided by the participants

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S1.1. SPATIAL SCALING CHALLENGE REPORTS #1

SPATIAL SCALING CHALLENGE DESCRIPTION OF THE METHODS

This document provides the participant with a structured template to report the methods used to estimate each of the biophysical or physiological variables required by the Spatial Scaling Challenge. After completing your analysis, fill out this form briefly and concisely.

Then copy/move the completed document to the folder /3_SCC_results/ without modifying its name and execute the last part of any of the scripts provided (SSC_script.py/m/R) to generate the compressed file to be sent to the Spatial Scaling Challenge organizers.

1. DISCUSSION

Vegetation status diagnosis

*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended)

The results of the variables estimated shows that for all variables the crops have a gradient of the values from North to South. For instance, LAI values obtained in the Field 1 shows values between 4 and 6 obtaining the higher values at the north of the field and the lower values at the south. In the case of the Field 2 the values range from 3.5 to 7, also obtaining higher values at the north than the south. This behaviour is the same in case of chlorophyll and Vcmax variables. In case of NPQ an inverse gradient is obtained with higher values in the south and lower values in the north. These results show that the crops are more efficient at the north of the fields and the south of the fields contains more stressed plants.

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Partial least squares regression (PLSR)

*Which type of method do you use? (Remove those that do not apply)

1: Statistical

*Which are the input parameters or predictors of the algorithm?

Hemispherical Directional Reflectance Factor (HDRF)

Sun-induced chlorophyll fluorescence radiance (F)

Land surface temperature (LST)

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

For the retrieval of LAI variable, the machine learning regression algorithm PLSR was used. It is a technique that reduces the predictor variables to a smaller set of factors. Then, a regression is performed using these reduced factors. For the training of the model we used the 18 field points.

Uncertainties were obtained using bootstrapping technique. It consists of the train model with 100 different randomly permutated subsets of the original dataset. Each subtrain is performed using 66% of the dataset size. Once trained the 100 submodels, we can obtain the mean of the predictions and the standard deviation of the predicted values as an estimation of the model uncertainty.

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Kernel ridge regression (KRR)

*Which type of method do you use? (Remove those that do not apply)

1: Statistical

*Which are the input parameters or predictors of the algorithm?

Hemispherical Directional Reflectance Factor (HDRF)

Sun-induced chlorophyll fluorescence radiance (F)

Land surface temperature (LST)

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

For the retrieval of Leaf chlorophyll content, the machine learning regression algorithm KRR was used. It is a nonlinear version of ridge regression through kernel functions. Because of its simplicity, KRR is very fast in training and running while maintaining competitive retrieval performances.

In this case, I performed an input dimensional reduction using Principal Component Analysis (PCA). It is a linear dimensional reduction technique that is used to reduce the number of dimensions in the dataset. PCA reduces the dataset dimension projecting the original spectra into a set of vectors, or principal components, that account for the largest amounts of variation in the data set. This is done by obtaining the eigenvectors and eigenvalues of the estimated covariance matrix of the spectral inputs.

Uncertainties were obtained using bootstrapping technique. It consists of train the model with 100 different randomly permutated subsets of the original dataset. Each subtrain is performed using 66% of the dataset size. Once trained the 100 submodels, we can obtain the mean of the predictions and the standard deviation of the predicted values as an estimation of the model uncertainty.

Leaf maximum carboxylation rate at 25 ºC ($V_{cmax,25}$, [µmol CO_2 cm^{-2} s^{-1}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Kernel ridge regression (KRR)

*Which type of method do you use? (Remove those that do not apply)

1: Statistical

*Which are the input parameters or predictors of the algorithm?

Hemispherical Directional Reflectance Factor (HDRF)

Sun-induced chlorophyll fluorescence radiance (F)

Land surface temperature (LST)

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

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In this case, I performed an input dimensional reduction using Principal Component Analysis (PCA). It is a linear dimensional reduction technique that is used to reduce the number of dimensions in the dataset. PCA reduces the dataset dimension projecting the original spectra into a set of vectors, or principal components, that account for the largest amounts of variation in the data set. This is done by obtaining the eigenvectors and eigenvalues of the estimated covariance matrix of the spectral inputs.

Uncertainties were obtained using bootstrapping technique. It consists of the train model with 100 different randomly permutated subsets of the original dataset. Each subtrain is performed using 66% of the dataset size. Once trained the 100 submodels, we can obtain the mean of the predictions and the standard deviation of the predicted values as an estimation of the model uncertainty.

Leaf non-photochemical quenching (*NPQ*, [-])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Partial least squares regression (PLSR)

*Which type of method do you use? (Remove those that do not apply)

1: Statistical

*Which are the input parameters or predictors of the algorithm?

Hemispherical Directional Reflectance Factor (HDRF)

Sun-induced chlorophyll fluorescence radiance (F)

Land surface temperature (LST)
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *For the retrieval of NPQ variable, the machine learning regression algorithm PLSR was used. It is a technique that reduces the predictor variables to a smaller set of factors. Then, a regression is performed using these reduced factors. For the training of the model we used the 18 field points.* *Uncertainties were obtained using bootstrapping technique. It consists of train the model with 100 different randomly permutated subsets of the original dataset. Each subtrain is performed using 66% of the dataset size. Once trained the 100 submodels, we can obtain the mean of the predictions and the standard deviation of the predicted values as an estimation of the model uncertainty.*

#2

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

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1. DISCUSSION

Vegetation status diagnosis

*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended)

Answer here

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Hybrid inversion using PROSPECT-D & SAIL models for simulation and support vector machine (SVM) as regression algorithm.

Reference using similar approach: Hauser et al., 2021

*Which type of method do you use? (Remove those that do not apply)

5: Other: hybrid inversion based on physical modeling and machine learning regression (SVM).

*Which are the input parameters or predictors of the algorithm?

Canopy reflectance is simulated based on the spectral response function of the sensor as provided.

Input parameters for PROSPECT-D and 4SAIL are either selected based on uniform distribution over a range defined by user, or set to a default value:

- *Leaf chlorophyll, carotenoid and brown pigments content, EWT, LMA, leaf structure parameter randomly assigned*
- *Leaf anthocyanin content set to 0*

- *Soil properties defined based on a weighted average of a wet soil and dry soil (adjusted to data with NDVI thresholding to extract 'bare soil' spectra)*
- *Observer zenith angle and sun/observer azimuth randomly selected based on range defined for dataset.*
- *Sun zenith angle set between 25 and 35 degrees from vertical.*
- *Gaussian noise applied on simulated reflectance (5% relative reflectance for LAI)*

LAI values are randomly generated using an uniform distribution for values ranging between 0 and 6.5 m^2 m^{-2}

Predictors: Spectral range adjusted depending on parameter:

- *spectral bands > 710 nm for the estimation of LAI*

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

A set of 2000 canopy reflectance was simulated using PROSAIL. Noise was added. The spectral domain was adjusted to discard spectral bands <710 nm. The simulated dataset was split into 20 subsets of 100 samples. 20 SVM regression models were then trained on each individual subset. The SVM models were then applied on the test dataset in order to estimate LAI.

The estimated LAI reported here corresponds to the value averaged over 20 subsets

The corresponding uncertainty for each sample is the standard deviation over 20 subsets.

Reference using similar approach: (Hauser et al., 2021

All codes are based on functions implemented in the R package prosail (https://jbferet.gitlab.io/prosail/index.html) (Feret and de Boissieu, 2023)

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Hybrid inversion using PROSPECT-D & SAIL models for simulation and support vector regression as regression algorithm.

Reference using similar approach: Hauser et al., 2021

*Which type of method do you use? (Remove those that do not apply)

5: Other: hybrid inversion based on physical modeling and machine learning regression.

*Which are the input parameters or predictors of the algorithm?

Canopy reflectance is simulated based on the spectral response function of the sensor as provided.

Input parameters for PROSPECT-D and 4SAIL are either selected based on uniform distribution over a range defined by user, or set to a default value:

- *Leaf chlorophyll, carotenoid and brown pigments content, EWT, LMA, leaf structure parameter randomly assigned*
- *Leaf anthocyanin content set to 0*
- *Soil properties defined based on a weighted average of a wet soil and dry soil (adjusted to data with NDVI thresholding to extract 'bare soil' spectra)*
- *Observer zenith angle and sun/observer azimuth randomly selected based on range defined for dataset.*
- *Sun zenith angle set between 25 and 35 degrees from vertical.*
- *Gaussian noise applied on simulated reflectance (2.5% relative reflectance for leaf chlorophyll content)*

Leaf chlorophyll content values are randomly generated using an uniform distribution for values ranging between 10 and 80 µg² cm⁻²

Predictors: Spectral range adjusted depending on parameter:

- *spectral bands > 700 nm for the estimation of leaf chlorophyll content*

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

A set of 2000 canopy reflectance was simulated using PROSAIL. Noise was added. The spectral domain was adjusted to discard spectral bands <700 nm. The simulated dataset was split into 20 subsets of 100 samples. 20 SVM regression models were then trained on each individual subset. The SVM models were then applied on the test dataset in order to estimate leaf chlorophyll content.

The estimated chlorophyll content reported here corresponds to the value averaged over 20 subsets

The corresponding uncertainty for each sample is the standard deviation over 20 subsets.

Reference using similar approach: Hauser et al., 2021

All codes are based on functions implemented in the R package prosail (https://jbferet.gitlab.io/prosail/index.html) (Feret and de Boissieu, 2023)

Leaf maximum carboxylation rate at 25 ºC ($V_{cmax,25}$, [µmol CO_2 cm^{-2} s^{-1}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Hybrid inversion using PROSPECT-PRO & SAIL models for simulation and support vector machine (SVM) as regression algorithm.

Reference using similar approach: Hauser et al., 2021

*Which type of method do you use? (Remove those that do not apply)

5: Other: hybrid inversion based on physical modeling and machine learning regression. VcMax was estimated based on a linear regression model including second order polynomial estimates of leaf protein content and leaf chlorophyll content

*Which are the input parameters or predictors of the algorithm?

Canopy reflectance is simulated based on the spectral response function of the sensor as provided.

Input parameters for PROSPECT-PRO and 4SAIL are either selected based on uniform distribution over a range defined by user, or set to a default value:

- *Leaf chlorophyll, carotenoid and brown pigments content, EWT, leaf protein content, Carbon based constituent content, leaf structure parameter randomly assigned*
- *Leaf anthocyanin content set to 0*
- *Soil properties defined based on a weighted average of a wet soil and dry soil (adjusted to data with NDVI thresholding to extract 'bare soil' spectra)*
- *Observer zenith angle and sun/observer azimuth randomly selected based on range defined for dataset.*
- *Sun zenith angle set between 25 and 35 degrees from vertical.*
- *Gaussian noise applied on simulated reflectance (1.5% relative reflectance for leaf protein content)*
- *LAI was restricted to values between 3 and 6.5*

Leaf protein content values are randomly generated using an uniform distribution for values ranging between 0.0005 and 0.005 mg^2 cm^{-2}

Predictors: Spectral range adjusted depending on parameter:

- *spectral bands > 1540 nm for the estimation of leaf protein content*

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

A set of 2000 canopy reflectance was simulated using PROSAIL. Noise was added. The spectral domain was adjusted to discard spectral bands <700 nm for the estimation of leaf chlorophyll content and spectral bands <1540 nm for the estimation of leaf protein content. The simulated dataset was split into 20 subsets of 100 samples. 20 SVM regression models were then trained on each individual subset. The SVM models were then applied on the test dataset in order to estimate leaf chlorophyll content and leaf protein content.

The estimated chlorophyll content and protein content reported here corresponds to the value averaged over 20 subsets

The uncertainty corresponding to the polynomical model combining estimated proteins and chlorophylls was not computed. It could be possible based on the individual uncertainty related to the estimation of proteins and chlorophylls.

Reference using similar approach: Hauser et al., 2021

All codes are based on functions implemented in the R package prosail (https://jbferet.gitlab.io/prosail/index.html) (Feret and de Boissieu, 2023)

Leaf non-photochemical quenching (*NPQ*, [-])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Hybrid inversion using PROSPECT-PRO & SAIL models for simulation and support vector machine (SVM) as regression algorithm.

Reference using similar approach: Hauser et al., 2021

*Which type of method do you use? (Remove those that do not apply)

5: Other: hybrid inversion based on physical modeling and machine learning regression. VcMax was estimated based on a linear regression model including second order polynomial estimates of leaf chlorophyll content.

*Which are the input parameters or predictors of the algorithm?

Canopy reflectance is simulated based on the spectral response function of the sensor as provided.

Input parameters for PROSPECT-D and 4SAIL are either selected based on uniform distribution over a range defined by user, or set to a default value:

- *Leaf chlorophyll, carotenoid and brown pigments content, EWT, LMA, leaf structure parameter randomly assigned*
- *Leaf anthocyanin content set to 0*
- *Soil properties defined based on a weighted average of a wet soil and dry soil (adjusted to data with NDVI thresholding to extract 'bare soil' spectra)*
- *Observer zenith angle and sun/observer azimuth randomly selected based on range defined for dataset.*
- *Sun zenith angle set between 25 and 35 degrees from vertical.*

- *Gaussian noise applied on simulated reflectance (2.5% relative reflectance for leaf chlorophyll content)*

Leaf chlorophyll content values are randomly generated using an uniform distribution for values ranging between 10 and 80 µg^2 cm^{-2}

Predictors: Spectral range adjusted depending on parameter:

- *spectral bands > 700 nm for the estimation of leaf chlorophyll content*

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

A set of 2000 canopy reflectance was simulated using PROSAIL. Noise was added. The spectral domain was adjusted to discard spectral bands <700 nm for the estimation of leaf chlorophyll content and spectral bands <1540 nm for the estimation of leaf protein content. The simulated dataset was split into 20 subsets of 100 samples. 20 SVM regression models were then trained on each individual subset. The SVM models were then applied on the test dataset in order to estimate leaf chlorophyll content and leaf protein content.

The estimated chlorophyll content and protein content reported here corresponds to the value averaged over 20 subsets

The uncertainty corresponding to the polynomical model combining estimated proteins and chlorophylls was not computed. It could be possible based on the individual uncertainty related to the estimation of proteins and chlorophylls.

Reference using similar approach: Hauser et al., 2021

All codes are based on functions implemented in the R package prosail (https://jbferet.gitlab.io/prosail/index.html) (Feret and de Boissieu, 2023)

#3

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

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1. DISCUSSION

Vegetation status diagnosis
*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended) *The two crops have to be described more or less separately, although both showed an N to S trend of decreasing physiological activity, and increasing stress.*

2. METHODS

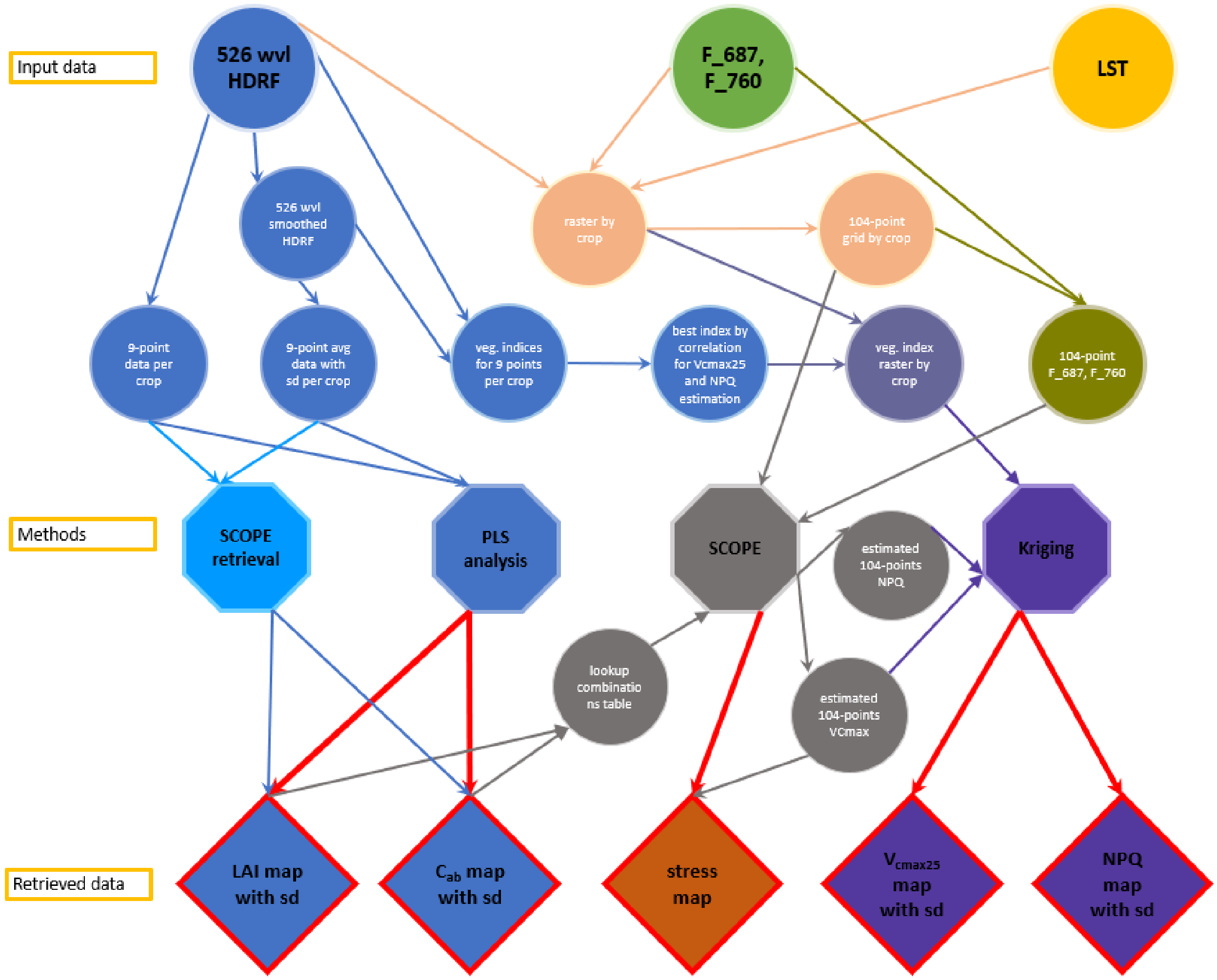

Figure 1: Mindmap of the process from input rasters to the maps of retrieved variables.

Leaf area index (*LAI*, [m^2 m^{-2}])
<u>*Provide the name of the approach/method/algorithm used (add literature reference if applicable)</u> *PLS analysis and SCOPE retrieval*
<u>**Which type of method do you use? (Remove those that do not apply)*</u> *2: Empirical (PLS) 4: Physically-based (SCOPE)*
<u>*Which are the input parameters or predictors of the algorithm?</u> *For PLS estimation, we used measured reflectance and during the process we selected wvl-s out of the 526 HDRF.* *For SCOPE retrieval, we used measured reflectance as input.*

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

For this estimation, we used on the one hand selected reflectance wvl-s out of the 526 HDRF bands based on PLS analysis. The selection procedure started with all bands (526) as input for the PLS model building and after the run the band with the lowest coefficient was left out from the input in the next model run until the number of bands reached 1. We extracted the corresponding wvl-s for different smoothness, but up-scaled to the same resolution (original raster, 1, 2, 4 and 8 m, smoothed rasters and sampled by pyramid image processing (Behrens et al., 2018)). The number (11 to 46) and wavelength of selected bands differed at different resolution input rasters. Then we summed the values of the selected wvl-s in a multiple linear regression model by the coefficients of the additive terms and intercept given by PLS. The output raster also differed in smoothness. The reason behind such an approach is that some ecological phenomena may have a different spatial scale from an underlying mechanism or a neighboring effect may act (Deng, 2007; Lassueur et al., 2006). The model with the lowest RMSEP value among different smoothness levels was used to map LAI and C_{ab} by also checking output averages and standard deviations for adequacy.

We also used SCOPE retrieval mode for the same purposes using all HDRF bands as input, however, the output showed a lower fit to the measured data, so our further steps were based on the PLS method.

Smoothing, sampling (by kernels), and then disaggregating rasters to the original resolution, instead of using point data is an adequate way to assess (mean) values and also standard deviations (sd) at different spatial scales. This approach is justified by an already differing spatial resolution of the input data (between 1-4 m for HDRF, F, and LST). PLS gave a set of coefficients for a good estimation of LAI and C_{ab} with a large R squared value for the 9 sampling positions and we also got sd values by using the same coefficients for error propagation which we calculated for the entire area of the two crops together with the estimated averages.

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

The same as for LAI.

**Which type of method do you use? (Remove those that do not apply)*

The same as for LAI.

*Which are the input parameters or predictors of the algorithm?

Same as for LAI, but always with a specific set of wvl-s from 526 HDRF bands differing from those used for LAI estimation and different for the scales (point, 1, 2, 4, 8 m).

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

Same as for LAI estimation.

Leaf maximum carboxylation rate at 25 °C (*$V_{cmax,25}$*, [µmol CO_2 cm^{-2} s^{-1}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *SCOPE model and spatial estimations*
**Which type of method do you use? (Remove those that do not apply)* *2: Empirical (Kriging) 4: Physically-based (SCOPE)*
*Which are the input parameters or predictors of the algorithm? *Maps of LAI and C_{ab}, lookup combination tables including possible Vcmax values (range for maize: 20-42/step:1, range for wheat: 10-54/step: 2) and F_687, F_760 for validation of the SCOPE model output. Vegetation index rasters derived from HDRF for kriging with external drift.*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *Selected point data from the LAI and C_{ab} rasters were used in SCOPE model for modeling SIF. In the first step we created 207 (23 V_{cmax25} * 3 LIDFa * 3 LIDFb) combinations of LAI, C_{ab}, V_{cmax25} and LIDF parameters for the. 104 spatial positions (which was found to result in a reasonable number of combinations in SCOPE). SCOPE model was run for each combinations for all of the spatial positions (1035 * 104). V_{cmax25} and NPQ output of the model runs were selected by minimizing the deviations of the modeled F_687 and F_760 values from the measured ones for each spatial position. This procedure was done for both crops and for both resolutions (1 m, 2 m).* *This number of output values as a spatial grid with additional refinement was adequate for further estimate target variables (V_{cmax25} and NPQ) for the entire area by means of kriging with external drift. Kriging is an interpolation technique for the estimation of the values of a variable at unsampled locations, based on the measured values in the neighbourhood. Universal kriging or kriging with external drift (KED) is a technique when the values of the sparsely measured target variable at unsampled locations are estimated based on a high resolution auxiliary variable (Oliver and Webster, 2014; Pebesma, 2004). In our study, vegetation indices derived from HDRF and checked for correlation with the original, measured V_{cmax25} and NPQ were used as the auxiliary variables. If KED kriging was not feasible we run ordinary kriging (OK), and if this one also failed, we used inverse distance weighting (IDW) for interpolation and mapping. Selection of appropriate output can be done by leave-one-out cross validation, but at this level of the analysis, we accepted maps with range of the values closest to the input field data. In this analysis, kriging variance served to assess local uncertainty.*

Leaf non-photochemical quenching (*NPQ*, [-])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *Same as for V_{cmax25}.*
*Which type of method do you use? (Remove those that do not apply) *2: Empirical (Kriging) 4: Physically-based (SCOPE)*
*Which are the input parameters or predictors of the algorithm?

Same as for V_{cmax25}.
<u>*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)</u> *Same as for V_{cmax25}.*

#4

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

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1. DISCUSSION

Vegetation status diagnosis

*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended)

Maize was generally less stressed than wheat as shown by relationships between i.e. NPQ2 vs nadir normalized (Hao et al., 2022) O2B band SIF (SIFB) values, and the higher LST and lower (also nadir normalised) O2Aband SIF (SIFA) values in wheat than in maize, respectively. O2B band yields (FiB) were lower and O2A band yields were higher in maize than in wheat suggesting stronger expression of stress in wheat. Stress was also shown in earlier NPQ values in wheat while in later ones and especially in NPQ2-NPQ1 differences in maize.

SIFB values were normalized by sunlit leaf area (SIFB_sl, obtained by retrieving leaf angle distribution factors from the SCOPE model first, then calculating the sunlit leaf area by using the retrieved LIDF values) assuming that the SIFB signal is dominated by sunlit leaf area. SIFB_sl showed the most negative correlations to both NPQ2 and NPQ1 in wheat, while in maize to their difference (NPQ2-NPQ1). SIFB_sl was also a close proxy of O2B band fluorescence yields in both species. SIFB_sl and B band yield (fiB) showed stress at higher significance levels than SIFA and fiA.

The southern part of both the wheat and maize fields were more stressed, shown by the NS gradients in LAI and Cab values and also by similar gradients in NPQ and Vcmax values shown on maps of these variables. There was also a (probably management-related) stress gradient present in the East-West direction, shown on the SIFB_sl map and on the combined (Vcmax, NPQ2, nadir normalized O2B and O2A yields) stress map. The North-South gradient seems to be continuous, while the perpendicular one is probably reflecting doses/different management stripes. The NS stress gradient was not present, however, on the fluorescence yield maps – these maps show the EW gradients, only.

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *The machine learning algorithm partial least squares regression was used from the pls package of R (Liland et al., 2022) after selecting variables on the base of their relative importance (mdatools package from R (Kucheryavskiy, 2023)) in the case of all four variables.*
*Which type of method do you use? (Remove those that do not apply) 1: Statistical 4: Physically-based
*Which are the input parameters or predictors of the algorithm? *Reflectance indices were selected on the base of their relative importance in PLSR.* *Wheat: PRI, MTCI, NDVI, NIRv, NDRE, CVI, FCVI, LST* *Maize: MTCI, NDVI, NIRv, NDRE, CVI, VIgreen, FCVI*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *The following reflectance indices were calculated from the reflectance data: PRI, NPQI, MTCI, RVSI, NDVI, NIRv, NDRE, CVI, VIgreen, FCVI. In addition to these indices, LST was also used as input into the regression analysis, where the wheat and the maize field was considered separately.* *Partial least squares regression (PLSR) in the R language was used. The method consists of a principal component analysis followed by a multilinear regression on the target variable.* *The base for selecting the important variables was the VIP score (variable importance for projection, (Andersen and Bro, 2010), after consideration the VIP score threshold was selected as 0.75. Five principal components were kept, and the coefficients obtained from the PLSR were used to produce the map of LAI (the same methodology was followed for the other target variables). Outliers in the predicted matrixes (maps) were filtered by excluding values outside the mean ± 5 times the standard deviation range.*

Leaf chlorophyll content (C_{ab}, [μg cm^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *The same method was used as in the case of LAI.*
*Which type of method do you use? (Remove those that do not apply) 1: Statistical
*Which are the input parameters or predictors of the algorithm? *Wheat: PRI, MTCI, NDVI, NIRv, NDRE, CVI, FCVI* *Maize: MTCI, NDVI, NIRv, NDRE, CVI, VIgreen, FCVI*

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

The same method was used as in the case of LAI.

Leaf maximum carboxylation rate at 25 °C ($V_{cmax,25}$, [μmol CO_2 cm^{-2} s^{-1}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

The same method was used as in the case of LAI.

*Which type of method do you use? (Remove those that do not apply)

1: Statistical

*Which are the input parameters or predictors of the algorithm?

Wheat: PRI, MTCI, NDVI, NIRv, NDRE, CVI, FCVI

Maize: NPQI, MTCI, NDVI, NIRv, NDRE, CVI, VIgreen, FCVI

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

The same method was used as in the case of LAI.

Leaf non-photochemical quenching (*NPQ*, [-])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

The same method was used as in the case of LAI.

*Which type of method do you use? (Remove those that do not apply)

1: Statistical

*Which are the input parameters or predictors of the algorithm?

Wheat: PRI, MTCI, RVSI, NDVI, NDRE, VIgreen

Maize: MTCI, RVSI, NDVI, NDRE, CVI, VIgreen, LST

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

The same method was used as in the case of LAI.

#5

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

This document provides the participant with a structured template to report the methods used to estimate each of the biophysical or physiological variables required by the Spatial Scaling Challenge. After completing your analysis, fill out this form briefly and concisely.

Then copy/move the completed document to the folder /3_SCC_results/ without modifying its name and execute the last part of any of the scripts provided (SSC_script.py/m/R) to generate the compressed file to be sent to the Spatial Scaling Challenge organizers.

1. DISCUSSION

Vegetation status diagnosis
*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended) All retrieved parameters display a clear south-north gradient. Lower Cab, LAI and Vcmax, and higher NPQ values suggest stronger stress of the plants in the southern part of both fields. Lowered LAI and Cab indicate slower growth due to long-term stress probably caused by different soil types and lower nitrogen and water content possibly associated with it. Based on the retrieved NPQ, wheat plants were experiencing stronger stress than maize. This can be explained by the lower temperature tolerance of wheat and the high temperature during the measurement period. Stronger stress of wheat is indicated also by higher variability of Vcmax in the wheat field than maize field. Vcmax of wheat was not strongly correlated with Cab content while Vcmax of maize was well correlated with Cab content. This suggests that a combination of long-term and acute stress caused damage in the photosynthetic apparatus of wheat plants while maize seems to be more tolerant.

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) SVM trained with ground-based data, HDRF bands with a correlation with LAI higher than 0.7, SIF 687 nm and 760 and LST
*Which type of method do you use? (Remove those that do not apply) 2: Empirical

*Which are the input parameters or predictors of the algorithm?

HDRF, SIF, LST and ground-based data

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

The HDRF spectrum was smoothed using a 5-step weighted moving average for each pixel. Once smoothed, from 1354 to 1520 nm and from 1717 to 2001.2 nm were replaced by the original data as there was no noise observed in that part. Smoothed spectra together with the rest of the airborne data were extracted for the points used for ground-based data and the correlation with LAI was used as a filter to reduce the number of bands from HDRF (R2>0.7). Each field was analyzed separately and two SVM models were created. Finally, the model was applied to the rest of the field making use of the airborne data. As no point from the soil was introduced, values of HDRF 680 nm higher than 0.15 were used to correct soil values. Only the RMSE from the model is provided as uncertainty.

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

SVM trained with ground-based data, HDRF bands with a correlation with Cab higher than 0.7, SIF 687 nm and 760 and LST

*Which type of method do you use? (Remove those that do not apply)

2: Empirical

*Which are the input parameters or predictors of the algorithm?

HDRF, SIF, LST and ground-based data

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

The HDRF spectrum was smoothed using a 5-step weighted moving average for each pixel. Once smoothed, from 1354 to 1520 nm and from 1717 to 2001.2 nm were replaced by the original data as there was no noise observed in that part. Smoothed spectra together with the rest of the airborne data were extracted for the points used for ground-based data and the correlation with C_{ab} was used as a filter to reduce the number of bands from HDRF (R2>0.7). Each field was analyzed separately and two SVM models were created. Finally, the model was applied to the rest of the field making use of the airborne data. As no point from the soil was introduced, values of HDRF 680 nm higher than 0.15 were used to correct soil values. Only the RMSE from the model is provided as uncertainty.

Leaf maximum carboxylation rate at 25 ºC ($V_{cmax,25}$, [µmol CO_2 cm^{-2} s^{-1}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

SVM trained with ground-based data, HDRF bands with a correlation with Vcmax higher than 0.7, SIF 687 nm and 760 and LST
*Which type of method do you use? (Remove those that do not apply) 2: Empirical
*Which are the input parameters or predictors of the algorithm? HDRF, SIF, LST and ground-based data
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) The HDRF spectrum was smoothed using a 5-step weighted moving average for each pixel. Once smoothed, from 1354 to 1520 nm and from 1717 to 2001.2 nm were replaced by the original data as there was no noise observed in that part. Smoothed spectra together with the rest of the airborne data were extracted for the points used for ground-based data and the correlation with Vcmax was used as a filter to reduce the number of bands from HDRF (R2>0.65). Each field was analyzed separately and two SVM models were created. Finally, the model was applied to the rest of the field making use of the airborne data. As no point from the soil was introduced, values of HDRF 680 nm higher than 0.15 were used to correct soil values. Only the RMSE from the model is provided as uncertainty.

Leaf non-photochemical quenching (*NPQ*, [-])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) SVM trained with ground-based data, HDRF bands with a correlation with Vcmax higher than 0.7, SIF 687 nm and 760 and LST
*Which type of method do you use? (Remove those that do not apply) 2: Empirical
*Which are the input parameters or predictors of the algorithm? HDRF, SIF, LST and ground-based data
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) The HDRF spectrum was smoothed using a 5-step weighted moving average for each pixel. Once smoothed, from 1354 to 1520 nm and from 1717 to 2001.2 nm were replaced by the original data as there was no noise observed in that part. Smoothed spectra together with the rest of the airborne data were extracted for the points used for ground-based data and the correlation with NPQ was used as a filter to reduce the number of bands from HDRF (R2>0.7). Each field was analyzed separately and two SVM models were created. Finally, the model was applied to the rest of the field making use of the airborne data. As no point from the soil was introduced, values of HDRF 680 nm higher than 0.15 were used to correct soil values. Only the RMSE from the model is provided as uncertainty.

#6

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

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1. DISCUSSION

Vegetation status diagnosis

*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended)

Looking at the predicted data, a clear difference in Cab is observed between the two fields.In maize Cab was predicted higher than in wheat. A clear gradient was observed in y-direction (north- south) of the plots, exhibiting higher Cab in the north gradually decreasing towards the south. Similar behavior was observed in predicted LAI and Vcmax. Predicted NPQ behaved inverse to the described above, with higher values in the wheat than in the corn, gradually increasing from north to south. With respect to the NPQ-time-series recorded in the northern parts of the plots, the predicted distinction between the corn and the wheat field is considered meaningful. The time series indicate photosynthesis adjusting to PAR in both fields, while maize shows a striking co-variation with air temperature in the morning. Thus it is followed, that the relatively low predicted NPQ in the maize field together with the relatively high Vcmax indicates a high photosynthetic activity. Maize as a C4 plant is coping well with the heat of the day around 36°C. On the contrary in the wheat field, relatively higher NPQ and lower Vcmax suggest a reduced photosynthetic activity. A strong gradient of further reduced photosynthesis towards the south is observed, which is supposed to coincide with a reduced canopy density as LAI is decreasing in both fields towards the south. The systematic difference in LST, exhibiting significantly higher temperatures in the wheat canopy compared with the maize canopy indicates reduced evapotranspiration in the wheat as a result of water-stress.

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

(Dayal and MacGregor, 1997)

Kernel-PLS: Dayal, B. S. and MacGregor, J. F. (1997) Improved PLS algorithms. Journal of Chemometrics, 11, 73–85. https://doi.org/10.1002/(SICI)1099-128X(199701)11:1<73::AID-CEM435>3.0.CO;2-%23

*Which type of method do you use? (Remove those that do not apply)

1: Statistical X 2: Empirical 3: Semi-empirical/Hybrid 4: Physically-based 5: Other (*describe*)

*Which are the input parameters or predictors of the algorithm?

A combined matrix of hyperspectral reflectance, land surface temperature, fluorescence and LAI in each ground-sampling point (530 variables for 18 instances) was used to train the algorithm. A combined list of hyperspectral reflectance, land surface temperature and fluorescence was used as predictor variables in each pixel of the airborne images.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

In each position of ground-measurements were hyperspectral reflectance (HDRF), sun-induced chlorophyll fluorescence (F) and land surface temperature (LST) extracted from the corresponding pixel of the airborne image. The positions of the ground sampling points were associated with the corresponding pixels using the recorded x-coordinates and y-coordinates. A large matrix with 530 variables was created, containing all extracted hyperspectral HDRF, F and LST values as well as the ground-sampled LAI values with respect to the 18 ground sampling points as instances.

The large (18 by 530) matrix was supplied as a training dataset to produce a supervised model using Kernel-PLS algorithm (Dayal and MacGregor, 1997) with the caret package in R (Kuhn, 2008; Kuhn et al., 2023)(Kuhn, 2008; Kuhn et al., 2021)*. The training was done using a 15-fold random cross-validation scheme with 10 repetitions. The optimal number of components was determined by optimizing for the lowest Root Mean Square Error (RMSE) during the cross-validation process. Best performed a model with $n = 3$ components and a corresponding error of $0.115\ m^2\ m^{-2}$. This RMSE error was assumed as the uncertainty value of the predicted LAI values.*

We combined HDRF, F and LST for each pixel position in the airborne images to use as predictor for the formerly trained Kernel PLS model using $n = 3$ components. The predicted LAI value was associated with the corresponding pixel position and stored as a new, virtual airborne image. The uncertainty expressed by the RMSE from the cross validation of the model was likewise stored as an airborne image.

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Kernel-PLS: Dayal and MacGregor, 1997

*Which type of method do you use? (Remove those that do not apply)

1: Statistical X 2: Empirical 3: Semi-empirical/Hybrid 4: Physically-based 5: Other (*describe*)

*Which are the input parameters or predictors of the algorithm?

A combined matrix of hyperspectral reflectance, land surface temperature, fluorescence and Cab in each ground-sampling point (530 variables for 18 instances) was used to train the algorithm. A combined list of hyperspectral reflectance, land surface temperature and fluorescence was used as predictor variables in each pixel of the airborne images.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

In each position of ground-measurements were hyperspectral reflectance (HDRF), sun-induced chlorophyll fluorescence (F) and land surface temperature (LST) extracted from the corresponding pixel of the airborne image. The positions of the ground sampling points were associated with the corresponding pixels using the recorded x-coordinates and y-coordinates. A large matrix with 530 variables was created, containing all extracted hyperspectral HDRF, F and LST values as well as the ground-sampled Cab values with respect to the 18 ground sampling points as instances.

The large (18 by 530) matrix was supplied as a training dataset to produce a supervised model using Kernel-PLS algorithm (Dayal and MacGregor, 1997) with the caret package in R (Kuhn, 2008; Kuhn et al., 2023)(Kuhn, 2008; Kuhn et al., 2021). *The training was done using a 15-fold random cross-validation scheme with 10 repetitions. The optimal number of components was determined by optimizing for the lowest Root Mean Square Error (RMSE) during the cross-validation process. Best performed a model with n = 3 components and a corresponding error of 1.23 µg cm*$^{-2}$. *This RMSE error was assumed as the uncertainty value of the predicted LAI values.*

We combined HDRF, F and LST for each pixel position in the airborne images to use as predictor for the formerly trained Kernel PLS model using n = 3 components. The predicted Cab value was associated with the corresponding pixel position and stored as a new, virtual airborne image. The uncertainty expressed by the RMSE from the cross validation of the model was likewise stored as an airborne image.

Leaf maximum carboxylation rate at 25 ºC ($V_{cmax,25}$, [µmol CO_2 cm^{-2} s^{-1}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Kernel-PLS: Dayal and MacGregor, 1997

*Which type of method do you use? (Remove those that do not apply)

1: Statistical X 2: Empirical 3: Semi-empirical/Hybrid 4: Physically-based 5: Other (*describe*)

*Which are the input parameters or predictors of the algorithm?

A combined matrix of hyperspectral reflectance, land surface temperature, fluorescence and Vcmax in each ground-sampling point (530 variables for 18 instances) was used to train the algorithm. A combined list of hyperspectral reflectance, land surface temperature and fluorescence was used as predictor variables in each pixel of the airborne images.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

In each position of ground-measurements were hyperspectral reflectance (HDRF), sun-induced chlorophyll fluorescence (F) and land surface temperature (LST) extracted from the corresponding pixel of the airborne image. The positions of the ground sampling points were associated with the corresponding pixels using the recorded x-coordinates and y-coordinates. A large matrix with 530 variables was created, containing all extracted hyperspectral HDRF, F and LST values as well as the ground-sampled Vcmax values with respect to the 18 ground sampling points as instances.

The large (18 by 530) matrix was supplied as a training dataset to produce a supervised model using Kernel-PLS algorithm (Dayal and MacGregor, 1997) with the caret package in R (Kuhn, 2008; Kuhn et al., 2023) (Kuhn, 2008; Kuhn et al., 2021). *The training was done using a 15-fold random cross-validation scheme with 10 repetitions. The optimal number of components was determined by optimizing for the lowest Root Mean Square Error (RMSE) during the cross-validation process. Best performed a model with n = 4 components and a corresponding error of 5.37 µmol CO_2 cm^{-2} s^{-1}. This RMSE error was assumed as the uncertainty value of the predicted LAI values.*

We combined HDRF, F and LST for each pixel position in the airborne images to use as predictor for the formerly trained Kernel PLS model using n = 4 components. The predicted Vcmax value was associated with the corresponding pixel position and stored as a new, virtual airborne image. The uncertainty expressed by the RMSE from the cross validation of the model was likewise stored as an airborne image.

Leaf non-photochemical quenching (*NPQ*, [-])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Kernel-PLS: Dayal and MacGregor, 1997

*Which type of method do you use? (Remove those that do not apply)

1: Statistical X 2: Empirical 3: Semi-empirical/Hybrid 4: Physically-based 5: Other (*describe*)

*Which are the input parameters or predictors of the algorithm?

A combined matrix of hyperspectral reflectance, land surface temperature, fluorescence and NPQ in each ground-sampling point (530 variables for 18 instances) was used to train the algorithm. A combined list of hyperspectral reflectance, land surface temperature and fluorescence was used as predictor variables in each pixel of the airborne images.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

In each position of ground-measurements were hyperspectral reflectance (HDRF), sun-induced chlorophyll fluorescence (F) and land surface temperature (LST) extracted from the corresponding pixel of the airborne image. The positions of the ground sampling points were associated with the corresponding pixels using the recorded x-coordinates and y-coordinates. A large matrix with 530 variables was created, containing all extracted hyperspectral HDRF, F and LST values as well as the ground-sampled Vcmax values with respect to the 18 ground sampling points as instances.

The large (18 by 530) matrix was supplied as a training dataset to produce a supervised model using Kernel-PLS algorithm (Dayal and MacGregor, 1997) with the caret package in R (Kuhn, 2008; Kuhn et al., 2023) (Kuhn, 2008; Kuhn et al., 2021). *The training was done using a 15-fold random cross-validation scheme with 10 repetitions. The optimal number of components was determined by optimizing for the lowest Root Mean Square Error (RMSE) during the cross-validation process. Best performed a model with n = 4 components and a corresponding error of 0.148. This RMSE error was assumed as the uncertainty value of the predicted LAI values.*

We combined HDRF, F and LST for each pixel position in the airborne images to use as predictor for the formerly trained Kernel PLS model using n = 4 components. The predicted NPQ value was associated with the *corresponding pixel position and stored as a new, virtual airborne image. The uncertainty expressed by the RMSE from the cross validation of the model was likewise stored as an airborne image.*

Classification and Regression Training. https://cran.r-project.org/web/packages/caret/index.html

#7

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

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1. DISCUSSION

Vegetation status diagnosis
*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended)   *Accurate quantification of photosynthetic and biochemical traits of vegetation are important for monitoring health and/or physiological status (Pacheco-Labrador et al., 2019). The V14 and booting stages in corn and wheat, respectively are the most critical growth stages of plant growth. These growth stages contain high amounts of green biomass which are closely linked to high leaf area index (LAI) ranged between 4 and 6.5. At these stages vegetation is highly sensitive to stress therefore any deficiency or injury to the plant can seriously impact crop yield and quality. For the given plots, the analysis results show that Vcmax ranges between 20-40 μmol·m^{-2}·s^{-1} which was lower than typical healthy vegetation (Camino et al., 2019; Wang et al., 2021b). Based on these results we conclude that both crops are under stress. There is a clear separation between the spatial distribution of Vcmax values of wheat and maize crops. Similar trend was followed with chlorophyll which is below the optimal range of 30-65 μg cm^{-2}. Based on these results, the stress could be related to water scarcity and nutrient deficiency. During this survey the temperature was 35^{0}C which accelerates transpiration and damages plant growth. The crops required immediate irrigation and fertigation for sustaining the growth.*

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *The retrieval of LAI of wheat and maize canopies using PROSAIL-PRO (Feret and de Boissieu, 2023) and gaussian process regression. We have utilized a hybrid approach to estimate LAI using a gaussian process regression algorithm and a look up table consisting of 1000 samples generated by PROSAIL-PRO. We have validated our model by using ground truth data provided and predicted LAI and uncertainty maps using the calibrated model.*
*Which type of method do you use? (Remove those that do not apply) Semi-empirical/Hybrid
*Which are the input parameters or predictors of the algorithm? *We have generated a look up table by using PROSAIL-PRO(Feret and de Boissieu, 2023). In order to generate the look up table we have constrained a number of parameters (e.g., Cab, solar geometry) by using the data provided. The following variables are considered in the simulation process.* *Structure parameter (N) : 1-3* *Chlorophyl a+b: 25-70* *Water thickness (Cw): 0.001-0.7* *Dry matter content (Cm): 0.0001-0.02* *Carotenoid content (Car): 0- 30* *Brown pigments (Cbrown): 0- 1* *Anthocyanins (Canth): 0- 10* *Protein content (Cp): 0-0.01* *Carbon based constituents 0.001-0.01* *Sun zenith angle 10-60* *View Zenith angle 0* *Average leaf inclination angle (ALIA) 30-70* *Soil brightness 0-1*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *We have generated a look up table using PROSAIL-PRO using a diverse range of leaf and canopy biophysical and biochemical variables. A total of 1000 combinations were generated from the input parameters. The LUT was then used to develop a model using gaussian process regression (GPR). GPR uses multiple non-parametric functions to correlate the spectral data with LAI. As we have large number of bands, we have used genetic algorithm to identify important bands. A regression model was developed using between simulated LAI values and simulated reflectance at selected bands. The model parameters were optimized using Bayesian algorithm. In addition to predictions, GPR provides uncertainty values for the estimates.*

Leaf chlorophyll content (C_{ab}, [μg cm^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *A hybrid method was used to retrieve leaf chlorophyll content in wheat and maize canopies. In the hybrid method leaf RTM PROSPECT-PRO and canopy RTM SAIL were coupled with gaussian process regression.*
*Which type of method do you use? (Remove those that do not apply) 3: Semi-empirical/Hybrid
*Which are the input parameters or predictors of the algorithm? *The leaf and canopy related variables were derived from PROSPECT-SAILH inversions. In which, the Cab and LAI variations were used based on ground data.* *The following variables considered in the simulation process.* *Structure parameter (N) : 1-3* *Chlorophyl a+b: 25-70* *Water thickness (Cw): 0.001-0.7* *Dry matter content (Cm): 0.0001-0.02* *Carotenoid content (Car): 0- 30* *Brown pigments (Cbrown): 0- 1* *Anthocyanins (Canth): 0- 10* *Protein content (Cp): 0-0.01* *Carbon based constituents 0.001-0.01* *Sun zenith angle 10-60* *View Zenith angle 0* *Average leaf inclination angle (ALIA) 30-70* *Soil brightness 0-1*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *A simulated training database was created using PROSPECT-PRO and 4SAIL models. A diverse range of leaf and canopy biophysical and biochemical were considered in the modelling process. A total of 1000 combinations were drawn from the input parameters. The LUT was then used to develop a model using gaussian process regression (GPR). GPR uses multiple non-paramteric functions to correlate the spectral data with leaf chlorophyll content. As we have large number of bands, we have used genetic algorithm to identify important bands. A regression model was developed using between simulated Cab values and simulated reflectance at selected bands. The model parameters were optimized using Bayesian algorithm. In addition to predictions, GPR provides uncertainty values for the estimates.*

Leaf maximum carboxylation rate at 25 °C ($V_{cmax,25}$, [µmol CO_2 cm^{-2} s^{-1}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

In this study, we have used a hybrid approach which leverages machine learning and SCOPE RTM simulations to retrieve Vcmax accurately.

*Which type of method do you use? (Remove those that do not apply)

3: Semi-empirical/Hybrid

*Which are the input parameters or predictors of the algorithm?

SCOPE simulations were carried out using a variety of input parameters, where the metrological data and other parameters were used from recorded field (air temperature, wind speed, incoming short and long wave infrared radiation, LAI, Chlorophyll)

The leaf and canopy related variables were derived from PROSPECT-SAIL inversions.

Cab (25-70),

Cw (0.001-0.05)

Cm((0.001-0.05),

LAI (2-6),LADF(1-4),

view zenith angle (0-20),

Vcmax (10-120),

M 8

Air pressure 970

wind speed 2-4

Air temperature(30-38),

Rin 300-900

Rli 300-390

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

The Vcmax used as a proxy to define the photosynthetic capacity of vegetation. High spectral resolution remote sensing data has potential to be used to estimate Vcmax at local and global scale through SCOPE model inversions (Zhang et al., 2014). In this study we have considered ground and metrological data for constraining the parameter distribution which can reduce ill-posed canopy radiative transfer inversion (Pacheco-Labrador et al., 2019). Using the above range of parameters, 1000 SCOPE simulations were built. From the simulations, bidirectional hemispherical reflectance spectra was considered in the modeling process. A GPR model was built between simulated spectra and corresponding Vcamax values. Similar to above process the model was optimized using

Bayesian approach. Since the retrieval of Vcmax is complex and function of multiple environment and canopy variables, the model is not very strong hence high uncertainty was noticed.

Leaf non-photochemical quenching (*NPQ*, [-])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Retrieval of NPQ using SIF values from the fluorescence imagery

*Which type of method do you use? (Remove those that do not apply)

Empirical

*Which are the input parameters or predictors of the algorithm?

Bayesian inference nonlinear regression between SIF and NPQ values

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

Sun induced fluorescence (SIF) can be used as a proxy for estimating NPQ. We obtained the SIF values at ground sampling locations and developed a regression equation between SIF (F687 and F760) and NPQ values. This equation was applied on the hyperspectral data cube for creating a spatial map. Along the predicted values, the associated uncertainty was estimated using Bayesian regression algorithm.

#8

SPATIAL SCALING CHALLENGE

DESCRIPTION OF THE METHODS

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1. DISCUSSION

Vegetation status diagnosis
*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended) *The LAI, Cab, Vcmax25 and NPQ were estimated.The observations that we can draw from the estimated biophysical variables are:* *For LAI estimates:* ✔ *There was not a common predictors to downscale LAI from canopy to leaf for the two crops (wheat and maize). LAI estimation was better for maize with R^2 = 0.94 and RMSE of 0.12 m^2 m^{-2}. The maps showed the spatial distribution of LAI depends on the foliage intensity coverage. Based on the maps, the bottom samples (12, 15 and 18 for maize and 3, 6 and 9 for wheat) demonstrated lower LAI values, which could be attributed to lower biomass.* *For Cab estimates:* ✔ *The observations draw on LAI estimates are also seeinable in Cab estimates.Cab estimated maps show that part of the maize and wheat located at the near the bottom of the maps (samples 3, 6, and 9 for wheat and 12, 15 and 18 for maize) are most likely affected by abiotic stresses such as water stress, as indicated with lowest Cab values.* *For Vcmax25 estimates:* ✔ *We observed a low prediction of Vcmax25 for wheat crop (R^2 = 0.66), compared to maize crop (R^2 = 0.91).Spatial patterns of the Vcmax25 estimates observed from the maps show high values of Vcmax25 from middle toward up and lower values in the bottom of the figures, suggesting that the crops located at the bottom of the maps may be affected by illumination stress or water stress.* *For NPQ estimates:* ✔ *We observed almost the same accuracy of NPQ estimates for maize and wheat using the red edge normalized difference vegetation index 2 (NDRE2) and the photochemical reflectance index (PRI). The spatial patterns of the NPQ maps showed low variations among the two crops but the NPQ values were greater at the bottom area of the maps, suggesting that the physiological status of the crops located from*

the bottom of the maps demonstrated some limitations for realizing photosynthesis, as part of the absorbed light are dissipated as heat.

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

We estimate LAI from reflectance-based vegetation indices, notably, the chlorophyll content index (Chl) and merris terrestrial chlorophyll index (MTCI), using an empirical linear regression model. For each crop type, we established a linear regression between LAI and Chl and MTCI for wheat and maize, respectively. The chlorophyll content index (Chl)(Gitelson et al., 2006), and the merris terrestrial chlorophyll index (MTCI) were computed as follows.

- ✔ *Chl* = $R_{750}/R_{700} - 1$*, where R is the reflectance at a given spectral wavelength (here at 750 nm and 700 nm).*
- ✔ *MTCI* = $(R_{800} - R_{710})/(R_{800} + R_{710})$.

*Which type of method do you use? (Remove those that do not apply)

2: Empirical

*Which are the input parameters or predictors of the algorithm?

LAI was predicted as function of MTCI for maize and Chl for wheat crop.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

Different reflectance-based vegetation indices were tested for LAI estimates. Based on the coefficient of determination (R^2) and the root mean squared error (RMSE) of the linear regressions, MTCI appears to be the best predictor of LAI for Maize, while the Chl is used to estimate LAI for wheat. The empirical linear regression between LAI and Chl and MTCI was used to map LAI at the canopy scales, but an uncertainty maps was not produced.

Equation used to derive LAI maps at the canopy scale:

LAI_maize = 14.26*MTCI - 3.42 ;

LAI_wheat = 0.57*Chl + 3.15.

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Cab estimates were achieved using empirical relationships from reflectance-based vegetation indices namely, Chl and the red edge normalized difference vegetation index 2 (NDRE2). The NDRE2 was computed following (Xie et al., 2019) : NDRE2 = $(R_{790} - R_{720})/(R_{790} + R_{720})$.

*Which type of method do you use? (Remove those that do not apply) 2: Empirical
*Which are the input parameters or predictors of the algorithm? Cab was estimated as function of NDRE2 for maize and Chl for wheat crop.
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) We applied the same method as describe in the LAI estimates. Linear regression equations: Cab_maize = 197.87*MTCI +18.49 . Cab_wheat = 6.33*Chl + 13.87.

Leaf maximum carboxylation rate at 25 ºC ($V_{cmax,25}$, [µmol CO_2 cm^{-2} s^{-1}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *The Vcmax25 was also estimated from reflectance-based vegetation indices such as the red edge normalized difference vegetation index (NDRE1) and Chl. The NDRE1 was calculated following Yu et al. (2014).* $NDRE1 = (R_{750} - R_{705})/(R_{750} + R_{705})$.
*Which type of method do you use? (Remove those that do not apply) 2: Empirical
*Which are the input parameters or predictors of the algorithm? *Answer here* Vcmax25 was predicted as function of NDRE1 for maize and Chl for wheat crop.
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *Answer here* The previous approaches used to derive canopy scales maps were used to map Vcmax25 at the canopy scale. However, it is worth mentioning that the uncertainty maps of Vcmax25 was not derived. Linear regression equations: Vcmax25_maize = 101.54*NDRE1 -35.67. Vcmax25_wheat = 15.32*Chl-37.65.

Leaf non-photochemical quenching (*NPQ*, [-])
<u>*Provide the name of the approach/method/algorithm used (add literature reference if applicable)</u> *Answer here* *The NPQ was also estimated from reflectance-based vegetation indices such as the NDRE2 and the photochemical reflectance index (PRI). PRI was calculated following (Gamon et al., 1992) Gamon et al. (1980).* *PRI = (R_{531}- R_{570})/ (R_{531}+R_{570}).*
<u>*Which type of method do you use? (Remove those that do not apply)</u> 2: Empirical
<u>*Which are the input parameters or predictors of the algorithm?</u> *Answer here* The PRI was used to estimate NPQ for wheat crop, while NDRE2 is used to estimate NPQ for maize.
<u>*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)</u> *Answer here* The NPQ maps were derived from the empirical relationships. However, it is worth mentioning that the uncertainty maps of NPQ was not derived. Linear regression equations: NPQ_maize = -2.37*NDRE2 + 0.85. NPQ_wheat = -7.54*Chl + 2.29.

#9

SPATIAL SCALING CHALLENGE

DESCRIPTION OF THE METHODS

This document provides the participant with a structured template to report the methods used to estimate each of the biophysical or physiological variables required by the Spatial Scaling Challenge. After completing your analysis, fill out this form briefly and concisely.

Then copy/move the completed document to the folder /3_SCC_results/ without modifying its name and execute the last part of any of the scripts provided (SSC_script.py/m/R) to generate the compressed file to be sent to the Spatial Scaling Challenge organizers.

1. DISCUSSION

Vegetation status diagnosis

*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended)

Answer here

We estimated LAI, Cab and Vcmax25. Unfortunately, we could not find a better way to predict NPQ.

The observations that we can draw from the estimated variables are:

For LAI estimates:

- ✔ *There was not a common predictors to upscale LAI from leaf to canopy for the two crops.*
- ✔ *LAI estimation was better for maize for both linear and multiple linear regression (R^2 = 0.94 and adj. R^2 = 0.94) vs for wheat(R^2 = 0.80 and adj. R^2 = 0.83).*
- ✔ *The maps shown that lowest LAI predictions was located among the bottom samples (12, 15 and 18 for maize and 3, 6 and 9 for wheat), whilst the best LAI prediction are found mostly in the samples located from middle to the up.*

For Cab estimates:

- ✔ *The observations draw on LAI estimates are also seeinable in Cab estimates.*
- ✔ *Cab results from the maps show that part of the maize and wheat located at the near the bottom of the maps (samples 3, 6, and 9 for wheat and 12, 15 and 18 for maize) are suffering from stress, as indicated with lowest Cab values.*

For Vcmax25 estimates:

- ✔ *We observed a low prediction of Vcmax25 for wheat crop (R^2 = 0.66 and adj. R^2 = 0.72), compared to maize crop (R^2 = 0.91 and adj. R^2 = 0.92).*
- ✔ *Spatial patterns of the Vcmax25 estimates observed from the maps show high values of Vcmax25 from middle toward up and lower values in the bottom of the figures, suggesting that the crops located at the bottom of the maps may suffer from stress.*

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *We estimate LAI from reflectance-based vegetation indices using a linear regression and multiple linear regression model. For each crop type, we established a linear and multiple linear regression model. We compute the chlorophyll content index (Chl) (Gitelson et al., 2006), the red edge normalized difference vegetation index 2 (NDRE2), and merris terrestrial chlorophyll index (MTCI).* *The formulations:* ✔ *Chl = R_750/R_700 – 1, where R is the reflectance at a given spectral wavelength (here at 750 nm and 700 nm).* ✔ *NDRE2 = (R_790-R_720)/(R_790+R_720) see (Xie et al., 2019).* ✔ *MTCI = (R_800-R_710)/(R_800+R_710).*
*Which type of method do you use? (Remove those that do not apply) 1: Statistical
*Which are the input parameters or predictors of the algorithm? For the linear regression, LAI is predicted as function of MTCI for maize and Chl for wheat crop, while for the multiple linear regression, NDRE2 and Chl are used as LAI predictors for maize crop, whilst Chl and R_700 are used to estimate LAI for wheat crop.
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) We tested first different reflectance-based vegetation indices for LAI estimates. Based on the coefficient of determination (R^2) and the root mean squared error (RMSE) of the linear regressions, MTCI appears to be the best predictor of LAI for Maize, while the Chl is used to estimate LAI for wheat. For the multi linear regression, NDRE2 and Chl are used to predict LAI for maize crop, whilst Chl and the reflectance at 700 nm are used to estimate LAI for wheat. We used the stats model ordinary least squares regression. The p value was statistically significant (<0.001). Linear regression equations: LAI_M = 14.26*MTCI - 3.42 for maize crop LAI estimate. LAI_W = 0.57*Chl + 3.15 for wheat crop LAI estimate. Multi linear regression equations: LAI_predict_m = 0.22*Chl+9.88*NDRE2 +2.56 for maize crop LAI estimate. LAI_predict_w = 0.06*Chl-56.95*R_700 +9.06 for wheat crop LAI estimate.

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *We also estimate Cab from reflectance-based vegetation indices and fluorescence ratio using a linear regression and multi linear regression model. For each crop type, we established a linear and multi linear regression model. We compute the fluorescence ratio (F-687/F-760) in addition to previous used vegetation indices.*
*Which type of method do you use? (Remove those that do not apply) 1: Statistical
*Which are the input parameters or predictors of the algorithm? For the linear regression, Cab is predicted as function of NDRE2 for maize and Chl for wheat crop, while for the multi linear regression, NDRE2, Chl and F_ratio are used as Cab predictors for maize, whearas F_ratio and Chl were used to estimate Cab for wheat crop.
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) We applied the same method as described in the LAI estimates. Linear regression equations: Cab_M = 197.87*MTCI +18.49 for maize crop. Cab_W = 6.33*Chl + 13.87 for wheat crop. Multiple linear regression equations: Cab_m = 99.67*NDRE2+4.25*Chl -8.43*F_ratio +12.47 for maize crop. Cab_w = 6.26*Chl -2.14*F_ratio+15.82 for wheat crop.

Leaf maximum carboxylation rate at 25 ºC ($V_{cmax,25}$, [µmol CO_2 cm^{-2} s^{-1}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *We also estimate Vcmax25 from reflectance-based vegetation indices and fluorescence ratio using a linear regression and multi linear regression model. For each crop type, we established a linear and multi linear regression model for each crop. We compute the normalized difference red edge index (NDRE1) and the near reflectance vegetation index (NIRv) in addition to previously used vegetation indices.* *NDRE1 = (R_750-R_705)/(R_750+R_705) see (*Yu et al., 2014*).* *NIRv = R_800*NDVI see (Badgley et al., 2017).* *NDVI = (R_800-R_680)/(R_800+R_680) see (*Yu et al., 2014*).*
*Which type of method do you use? (Remove those that do not apply) 1: Statistical

*Which are the input parameters or predictors of the algorithm? For the linear regression, Vcmax25 is predicted as function of NDRE1 for maize and Chl for wheat crop, while for the multi linear regression, NDRE1 and NDRE2 are used as Vcmax25 predictors for maize, whearas F_ratio, Chl and NIRv were used to estimate Cab for wheat crop.
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) The previous approaches were used in the section two. Linear regression equations: Vcmax25_M = 101.54*NDRE1 -35.67 for maize crop. Vcmax25_W = 15.32*Chl-37.65 for wheat crop. Multiple linear regression equations: Vcmax25_m = 64.14*NDRE1+28.94*MTCI-29.01 for maize crop. Vcmax25_w = 15.37*Chl+383.02*NIRv+29.84*F_ratio-197.85 for wheat crop.

Leaf non-photochemical quenching (*NPQ*, [-])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *Answer here*
*Which type of method do you use? (Remove those that do not apply) 1: Statistical 2: Empirical 3: Semi-empirical/Hybrid 4: Physically-based 5: Other (*describe*)
*Which are the input parameters or predictors of the algorithm? *Answer here*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *Answer here*

#10

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

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1. DISCUSSION

Vegetation status diagnosis
*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended) *I have evaluated the Water Deficit Index (WDI) proposed by (Moran et al., 1994) for crop water deficit using surface-air temperature and a spectral vegetation index (NDVI). The WDI index has been used to estimate evapotranspiration rates for mixed surfaces. WDI index reaches a value of 1 for conditions of extreme stress of the vegetation, and 0 for crop evaporation to its potential rate. From the results I can conclude that the plot on the right is ok while the one on the left is stressed (with an increasing gradient from bottom right to top left).*

2. METHODS

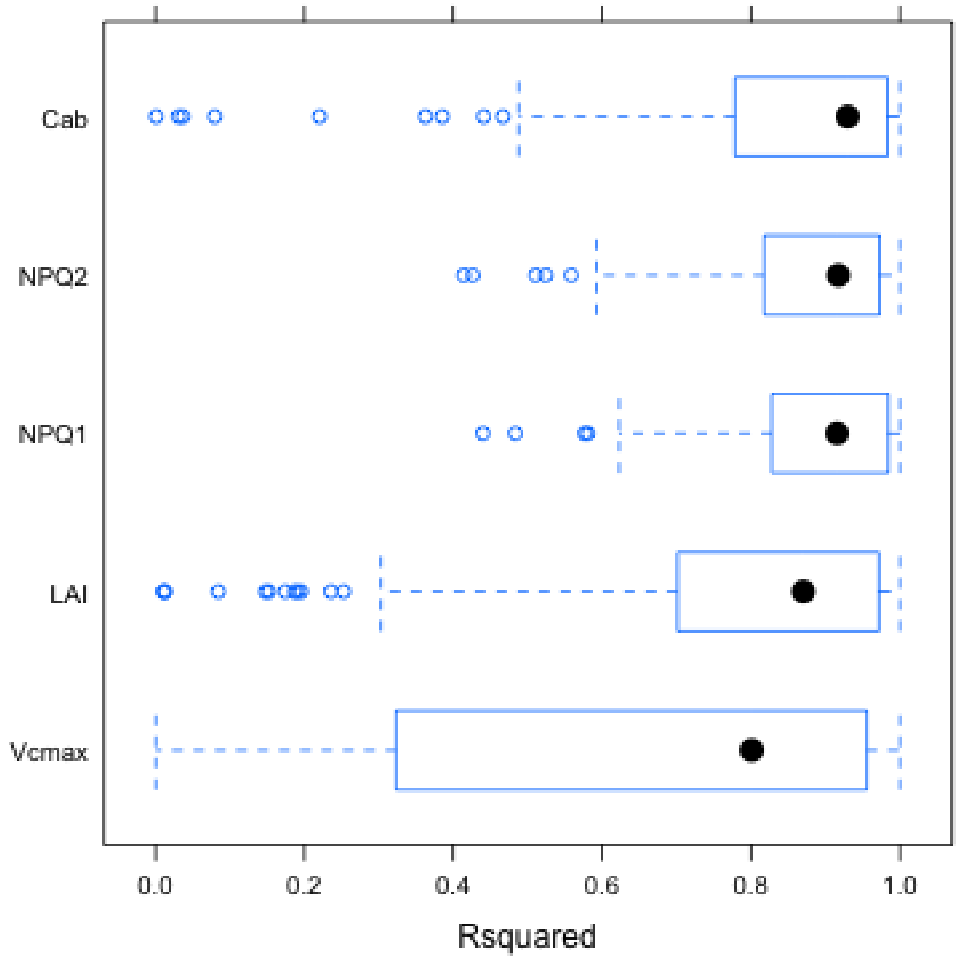
Leaf area index (*LAI*, [m^2 m^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *Breiman, 2001*
*Which type of method do you use? (Remove those that do not apply) 1: Statistical
*Which are the input parameters or predictors of the algorithm? *Fluorescence, LST and reflectances*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *I made use of Breiman's random forest algorithm with a 5 fold 10 times repeated cross-validation.*

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *Breiman, 2001*
*Which type of method do you use? (Remove those that do not apply) 1: Statistical
*Which are the input parameters or predictors of the algorithm? *Fluorescence, LST and reflectances*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *I made use of Breiman's random forest algorithm with a 5 fold 10 times repeated cross-validation.*

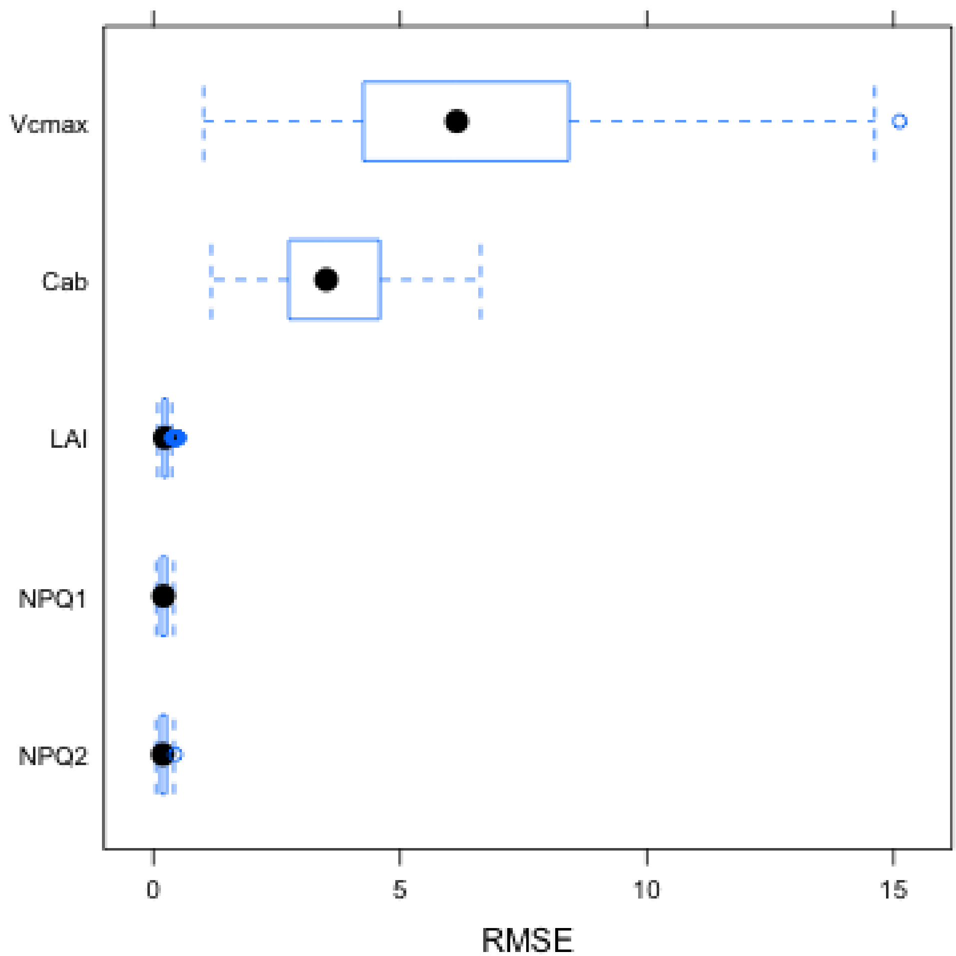
Leaf maximum carboxylation rate at 25 ºC ($V_{cmax,25}$, [µmol CO_2 cm^{-2} s^{-1}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *Breiman, 2001*
*Which type of method do you use? (Remove those that do not apply) 1: Statistical
*Which are the input parameters or predictors of the algorithm? *Fluorescence, LST and reflectances*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *I made use of Breiman's random forest algorithm with a 5 fold 10 times repeated cross-validation.*

Leaf non-photochemical quenching (*NPQ*, [-])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *Answer here*
*Which type of method do you use? (Remove those that do not apply)

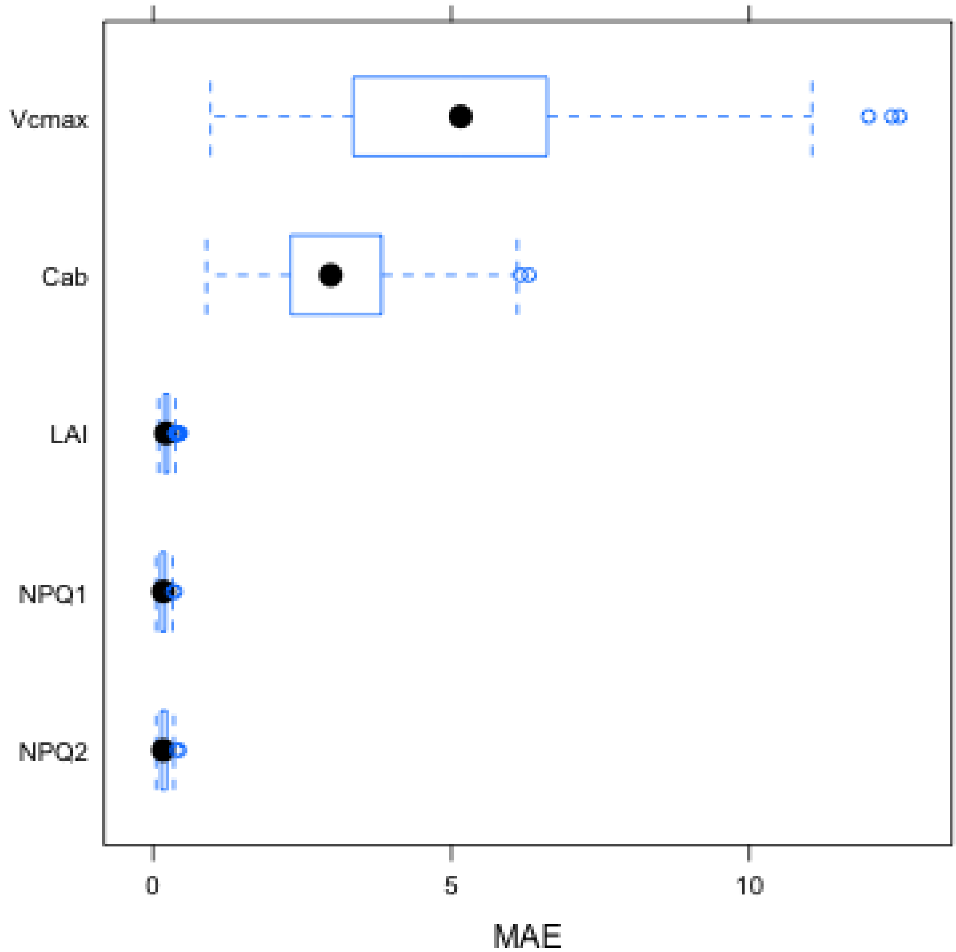
1: Statistical
*Which are the input parameters or predictors of the algorithm? *Fluorescence, LST and reflectances*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *I made use of Breiman's random forest algorithm with a 5 fold 10 times repeated cross-validation.*



Cab
NPQ2
NPQ1
LAI
Vcmax
0.0
0.2
0.4
0.6
0.8
1.0
Rsquared



Vcmax
Cab
LAI
NPQ1
NPQ2
0
5
10
15
RMSE



Vcmax
Cab
LAI
NPQ1
NPQ2
0
5
10
MAE

#11

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

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1. DISCUSSION

Vegetation status diagnosis
*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended) *Both plants seem well-developed, LAI and Cab are pretty hight. However, the Vcmax25 values are super low for agricultural crops (40 umol m-2 s-1, expected around 100 umol m-2 s-). This could be an adaptation to the hot Spanish conditions. NPQ at the time of the overpass was also quite high, at the end it was midday with 1000 W m-2 radiation and 33 degrees.For both crops, the most stressed fraction is at the bottom (south) of the images.*

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *Look-up table https://github.com/Prikaziuk/retrieval_rtmo (Prikaziuk, 2022)*
*Which type of method do you use? (Remove those that do not apply) 4: Physically-based
*Which are the input parameters or predictors of the algorithm? *Upper and lower boundaries of soil, leaf and canopy RTM parameters*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *Extracted 10 representative samples from reflectance bins* Fit with Numerical Optimization in the whole parameter space

Took the min and max values of retrieved parameters as look-up table boundaries Generated 1000 LUT spectra Retrieved. Wheat and Maize used different LUTs

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *Look-up table https://github.com/Prikaziuk/retrieval_rtmo (Prikaziuk, 2022)*
*Which type of method do you use? (Remove those that do not apply) 4: Physically-based
*Which are the input parameters or predictors of the algorithm? *Upper and lower boundaries of soil, leaf and canopy RTM parameters*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) *Extracted 10 representative samples from reflectance bins* Fit with Numerical Optimization in the whole parameter space Took the min and max values of retrieved parameters as look-up table boundaries Generated 1000 LUT spectra Retrieved. Wheat and Maize used different LUTs

Leaf maximum carboxylation rate at 25 °C ($V_{cmax,25}$, [µmol CO_2 cm^{-2} s^{-1}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) *Empirical linear correlation Vcmax25 = f(Cab)*
*Which type of method do you use? (Remove those that do not apply) 1: Statistical
*Which are the input parameters or predictors of the algorithm? *Measured Cab and Vcmax25*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

*Vcmax25 = 2.5 * Cab – 73, wheat (R2=0.70, RMSE=5.31 umol CO2 m-2 s-1)*
*Vcmax25 = 0.36 * Cab + 13.66, maiz (R2-0.9, RMSE=0.77 umol CO2 m-2 s-1)*

(Luo et al., 2019)

Leaf non-photochemical quenching (*NPQ*, [-])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

SCOPE

*Which type of method do you use? (Remove those that do not apply)

4: Physically-based

*Which are the input parameters or predictors of the algorithm?

Retrieved parameters + meteo at the time of overpass

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

Disclaimer: I have never worked with NPQ and did not really understand it in two weekend days. Curious to know the correct way of downscaling it. NPQ seems to strongly and almost linearly correlate with NDVI and PRI.

SCOPE.

NPQ defined as (Fm/Fm' – 1) is available for each sunlit (bcu) and shaded (bch) leaf but has not been directly written to SCOPE output files. I tweaked the model to write those data. The averaging manner is questionable: I used (1) plane average, kind of "mean sunlit leaf" [another option was the "meanleaf" function of scope, which outputs kind of "mean sunlit layer", that value was too low]. The total is the average of mean sunlit NPQ and mean shaded NPQ.

For wheat C3, for maize C4 photosynthesis type was used.

(van der Tol et al., 2014)

Van der Tol, C., J. A. Berry, P. K. E. Campbell, and U. Rascher. 2014. "Models of Fluorescence and Photosynthesis for Interpreting Measurements of Solar-induced Chlorophyll Fluorescence." Journal of Geophysical Research: Biogeosciences 119 (12): 2312–27. https://doi.org/10.1002/2014JG002713

#12

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

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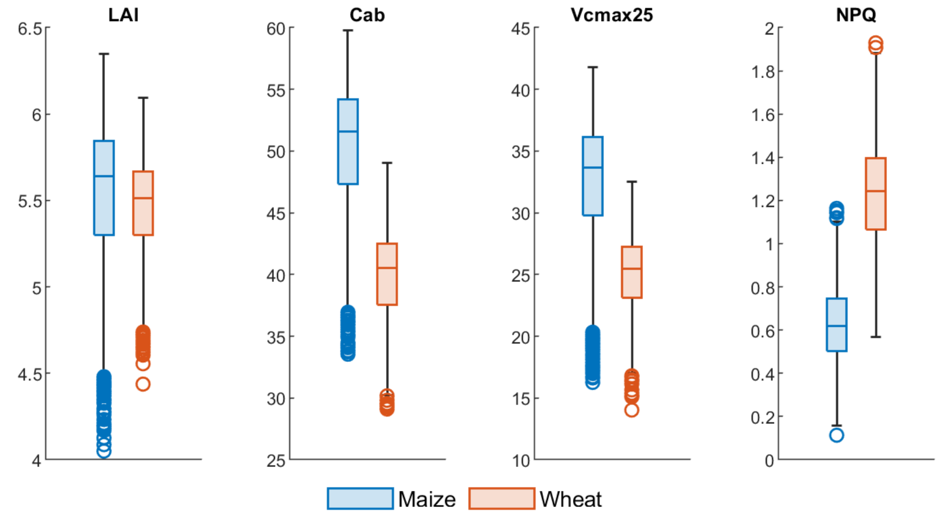
1. DISCUSSION

Vegetation status diagnosis

*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended)

For both crops, wheat and maize, a north-south gradient can be observed, which is visible for all traits except NPQ in the maize field. However, for all other traits, this gradient is more prominent for maize than for wheat. Values for LAI and leaf chlorophyll are higher in the northern zone which indicates less plant stress there. Higher LAI indicates that the plants are more developed in this part of the field, or in other words, vegetation growth is limited by some factors in the southern part. Higher leaf chlorophyll content indicates better nitrogen status or nitrogen availability in the soil. Both limitations, nutrient uptake and crop growth, can be caused by limited water availability. Since the gradient can be observed for both crops the morphology might cause this pattern. Heterogeneous soil conditions could also explain such gradients. Consequently, high radiation is leading to physiological stress on the southern part of the wheat plot which indicates lower water availability in this part of the field.

Temperatures in the wheat field are significantly higher than in the maize field so we can conclude that maize has a higher transpiration rate and is thus less stressed than the wheat, which is in agreement with the results of higher LAI, higher Vcmax25 and lower NPQ in the maize field (see box plots). The wheat seems to be unable to cool itself enough through transpiration and has thus to resort to non-photochemical quenching of the excess radiation. Furthermore, maize is a C4 crop in contrast to wheat (C3) and is less stressed by high radiation intensity.



2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) Partial Least Squares Regression (Wold et al., 2001) (PLSR, Wold et al. 2001). CWSI (Crop Water Stress Index) (Idso et al., 1981; Jackson et al., 1981)
*Which type of method do you use? (Remove those that do not apply) 1: Statistical 2: Empirical
*Which are the input parameters or predictors of the algorithm? We used different combinations of the following data sets: ● Reflectance (R) ● Fluorescence (F) ● Land Surface Temperature (LST) ● Crop Water Stress Index (CWSI) Reflectance was always part of the input data, so we had the combinations R; R & F; R & LST, R & CWSI; R, F & LST; R, F & CWSI; R, LST & CWSI; R, F, LST & CWSI. The CWSI is calculated as follows:

$$CWSI = 1 - \frac{ET_{act}}{ET_{pot}} = \frac{(T_c - T_a)_c - (T_c - T_a)_{ll}}{(T_c - T_a)_{ul} - (T_c - T_a)_{ll}}$$

CWSI (Crop Water Stress Index) is defined by the relationship between actual (ET_{act}) and potential (ET_{pot}) evaporation (Idso et al., 1981; Jackson et al., 1981). However, the physical-based CWSI requires many input data. A more simple and fast way is the calculation of the image-based CWSI. Usually one would use dry and wet targets in the field. However, since such targets have not been available, we calculated a simplified version of the image-based CWSI. Therefore, for each crop, the 5% for the warmest (=T_{dry}) and coolest (=T_{wet}) pixels have been extracted and averaged. Mixed pixels of the boundary zone have been avoided.

For wheat, the warmest (ul=upper limit) and coolest (ll=lower limit) 5% pixels showed values of 317.18 and 313.75 K respectively. For maize, values were 323.16 and 309.69 K. Air temperature was 308.75 K. Normalisation with air temperature is not explicitly necessary since it is a one-time study but for studies analyzing several time steps such normalization is recommended. The image-based CWSI was calculated following the formula: CWSI= $(T_c-T_{wet})/(T_{dry}-T_{wet})$, where T_c =temperature of the canopy.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

For each combination of input data, a PLSR with 5-fold cross-validation with up to 10 components (latent variables) was calculated 100 times. From the mean values of mean squared error, the optimal number of components for each combination of inputs was determined (figure 1).

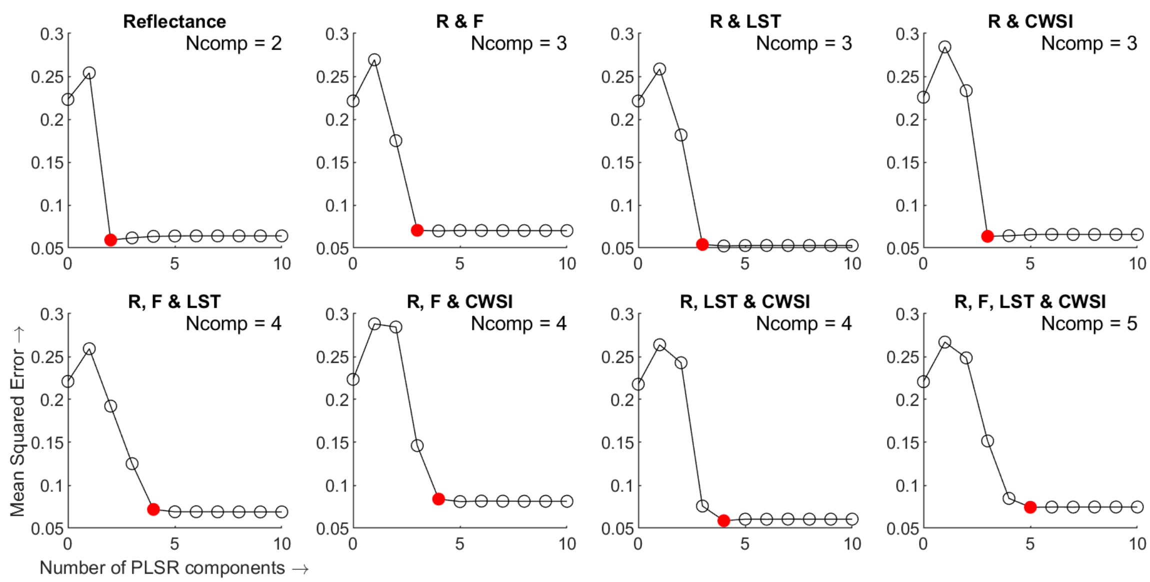


Figure 1: Mean Squared Error depending on the number of latent PLSR variables for each combination of inputs for estimation of LAI.

Using this optimal number, the PLSR was calculated for each combination of input variables. Figure 2 shows the relationship between measured to estimated values and the R² values. The model with the highest R² value was selected and applied to the image data to create a map (figure 3). Usually, one would recommend using two different models for the two crops. However, as figure 2 shows, the vegetation traits of the two crops show very similar behavior and data range which allows the combination and an increase in sample size.

To estimate uncertainty, a method similar to the one described by (Singh et al., 2015) Singh et al. (2015) was adopte
The PLSR was repeated 100 times with random subsets of two-thirds of the training data points. The standard devia
between these estimations is given as uncertainty in figure 3.

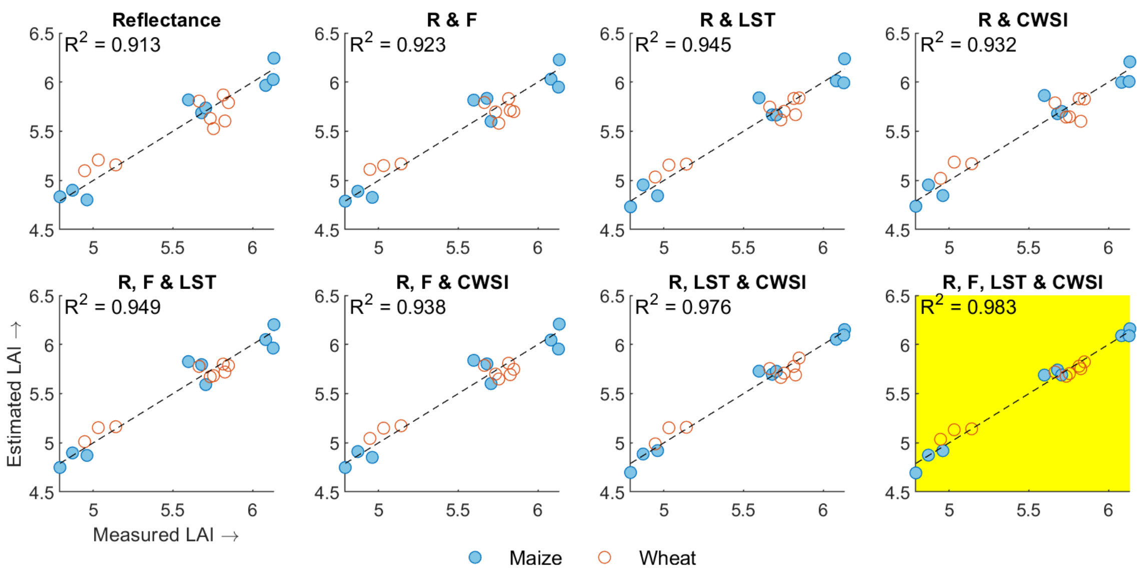


Figure 2: Estimation of LAI using different input combinations. The best model is marked in yellow.

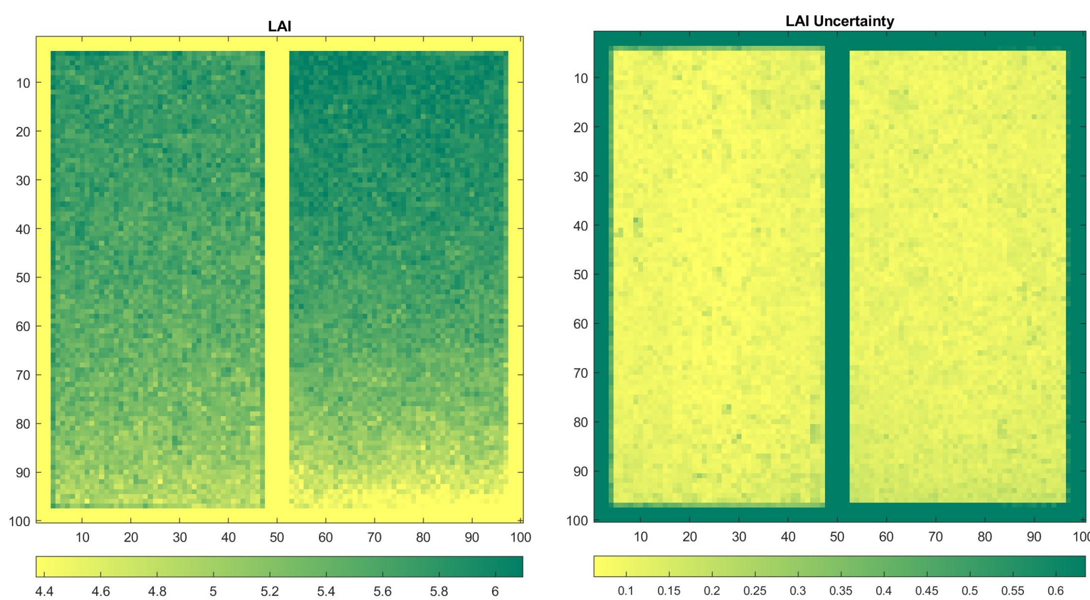


Figure 3: Left: Map of estimated LAI values (left parcel wheat, right maize). Right: Map of LAI uncertainties.

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Same approaches as LAI estimation

*Which type of method do you use? (Remove those that do not apply)

1: Statistical   2: Empirical

*Which are the input parameters or predictors of the algorithm?

See LAI section

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

We used the approach described in the LAI section.

Figure 4 shows the determination of the optimal number of components for each combination of inputs, figure 5 shows the scatter plots of measured versus estimated values for each input combination and figure 6 shows the resulting map and uncertainty map.

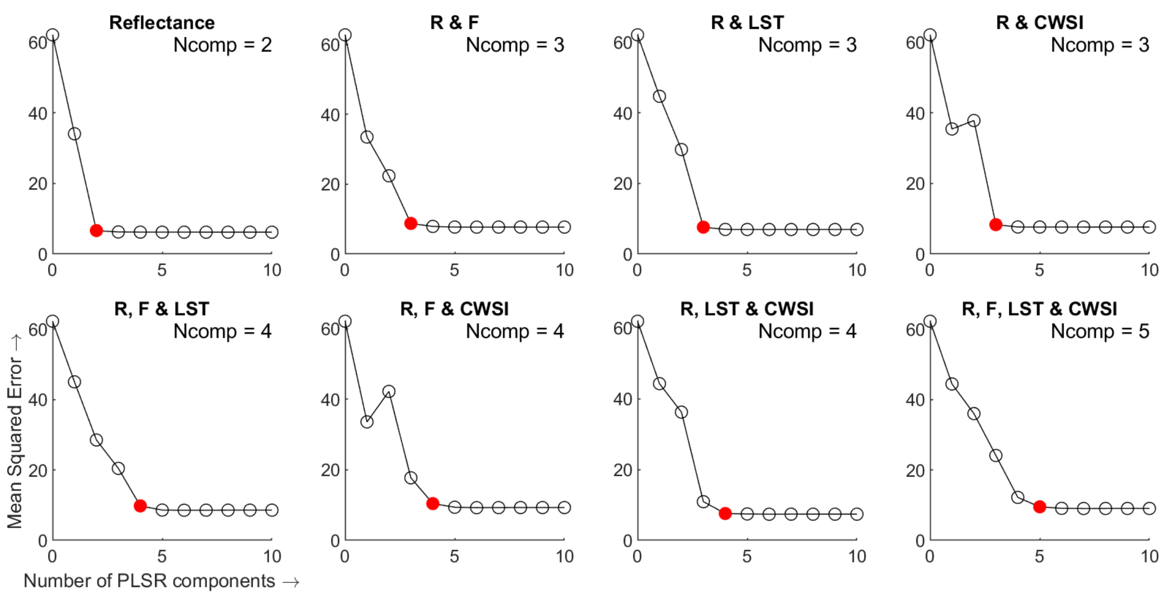


Figure 4: Mean squared error versus number of PLSR components to determine optimal number of components for each input combination for Cab.

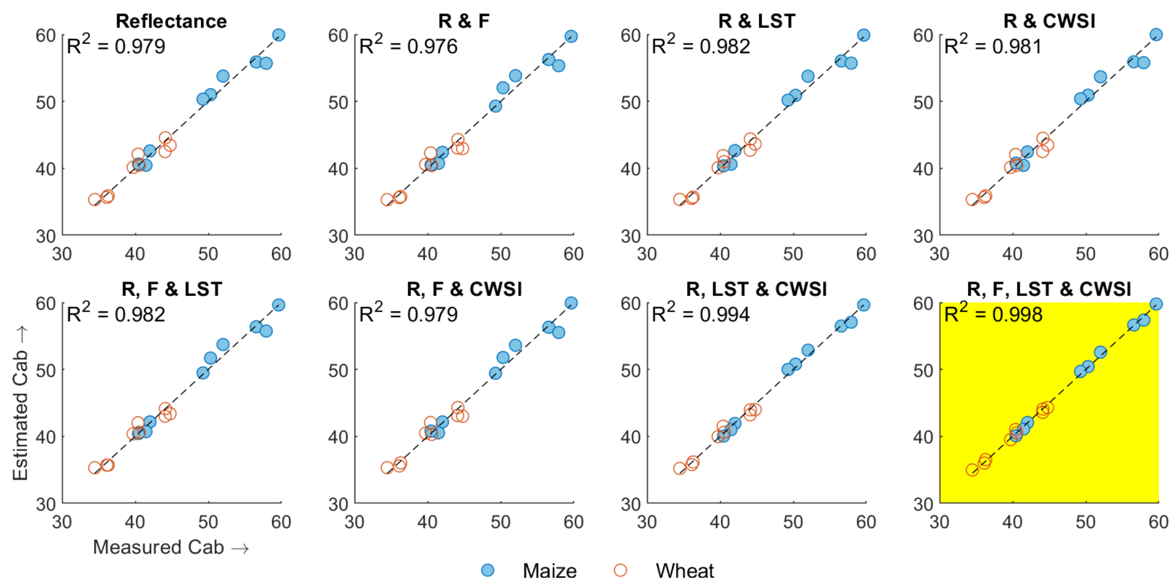


Figure 5: Scatterplots of measured versus estimated Cab for each input combination. The best variant is marked in yellow.

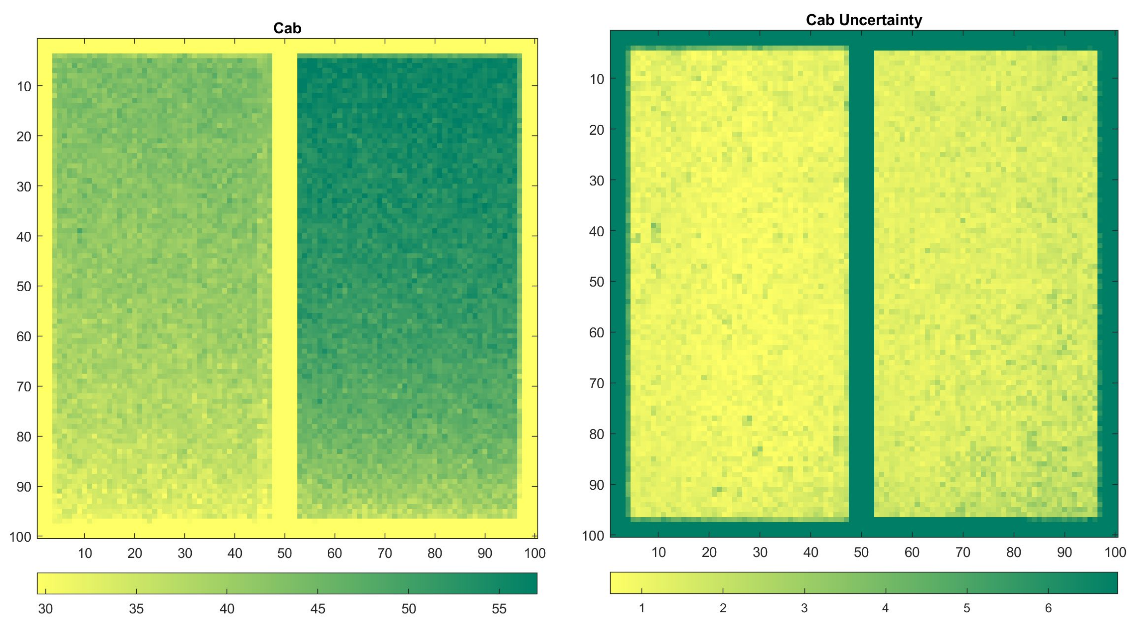


Figure 6: Resulting map and uncertainties.

Leaf maximum carboxylation rate at 25 °C ($V_{cmax,25}$, [μmol CO_2 cm^{-2} s^{-1}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

See LAI section

*Which type of method do you use? (Remove those that do not apply)

1: Statistical 2: Empirical

*Which are the input parameters or predictors of the algorithm?

See LAI section

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

We used the approach described in the LAI section.

Figure 7 shows the determination of the optimal number of components for each combination of inputs, figure 8 shows the scatter plots of measured versus estimated values for each input combination and figure 9 shows the resulting map and uncertainty map.

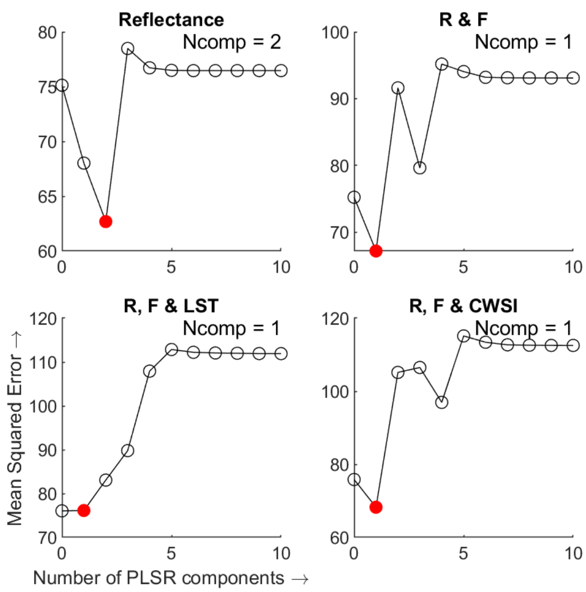


Figure 7: Mean squared error versus number of PLSR components to determine optimal number of components for each input combination for Vcmax.

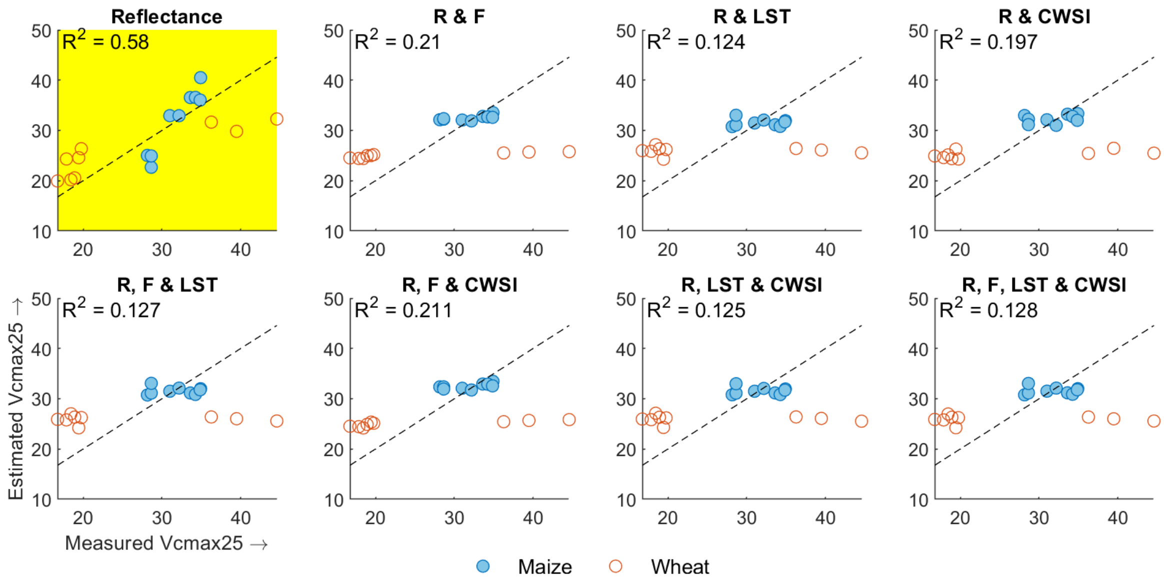


Figure 8: Scatterplots of measured versus estimated Vcmax for each input combination. The best variant is marked in yellow.

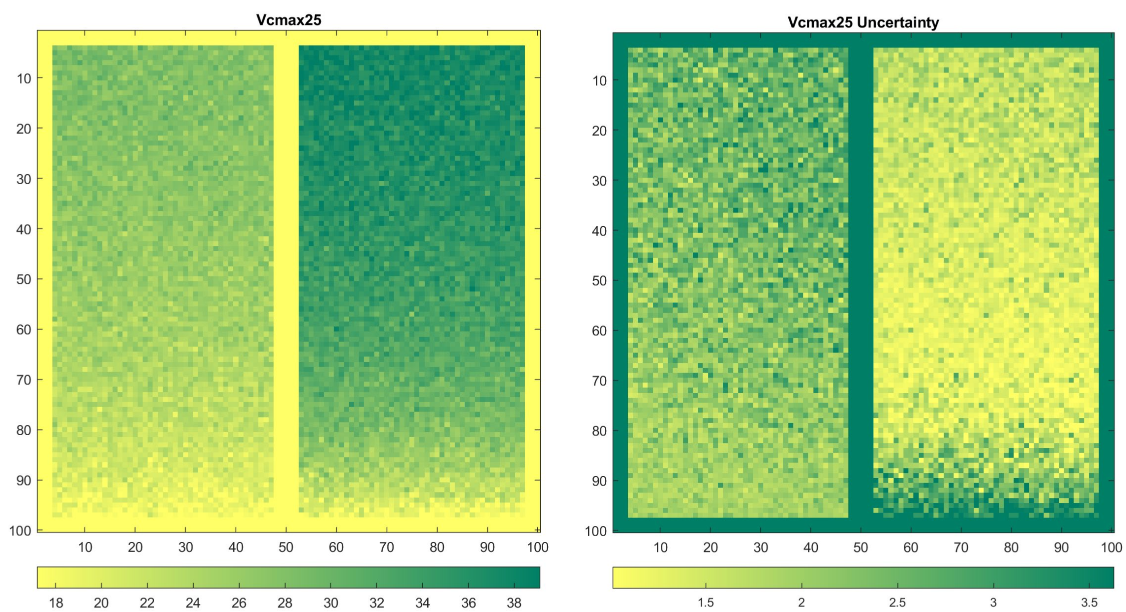
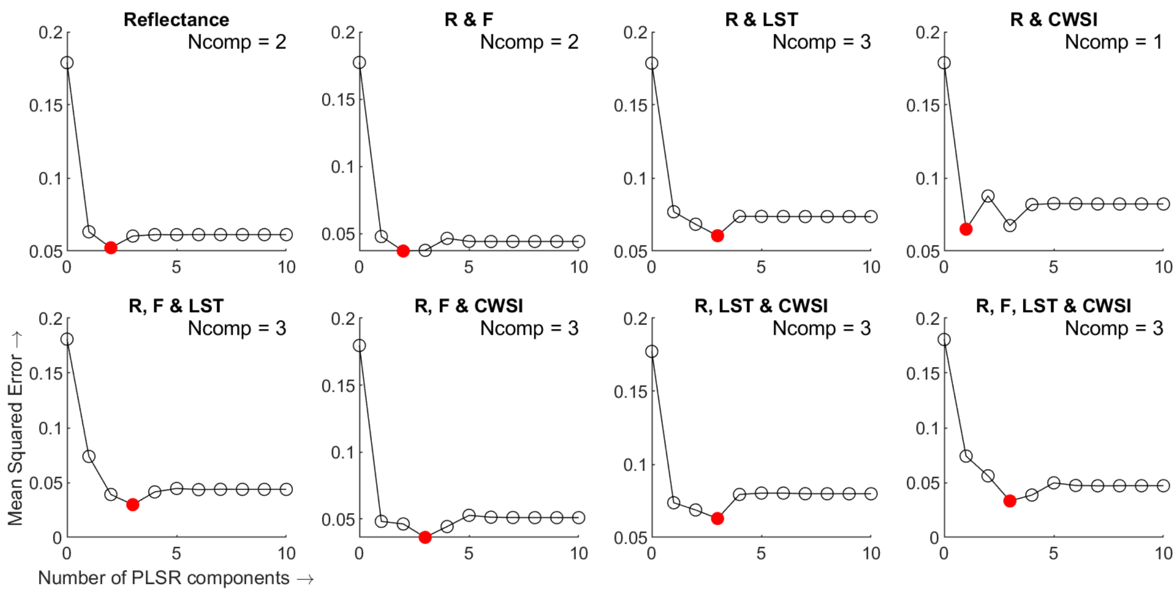


Figure 9: Resulting map and uncertainties.

Leaf non-photochemical quenching (*NPQ*, [-])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

See LAI section
*Which type of method do you use? (Remove those that do not apply) 1: Statistical 2: Empirical
*Which are the input parameters or predictors of the algorithm? *See LAI section*
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) We used the approach described in the LAI section, separately for NPQ1 and NPQ2. In the end, the maps were averaged to get the NPQ estimation. Figure 10 shows the determination of the optimal number of components for each combination of inputs, figure 11 shows the scatter plots of measured versus estimated values for each input combination and figure 12 shows the resulting trait and uncertainty maps. 

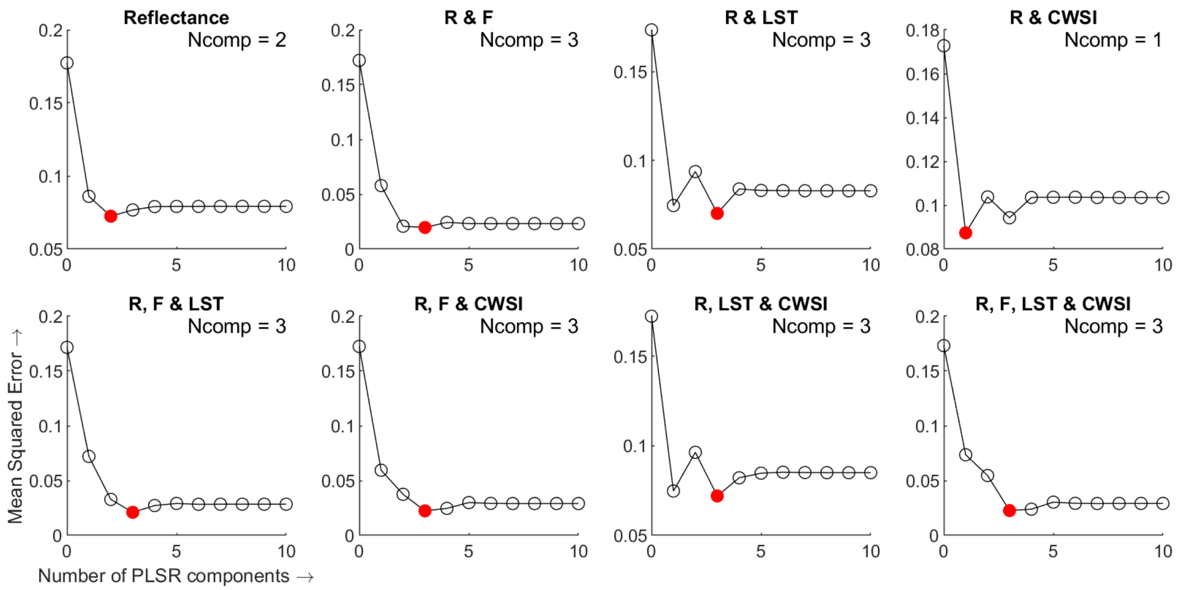
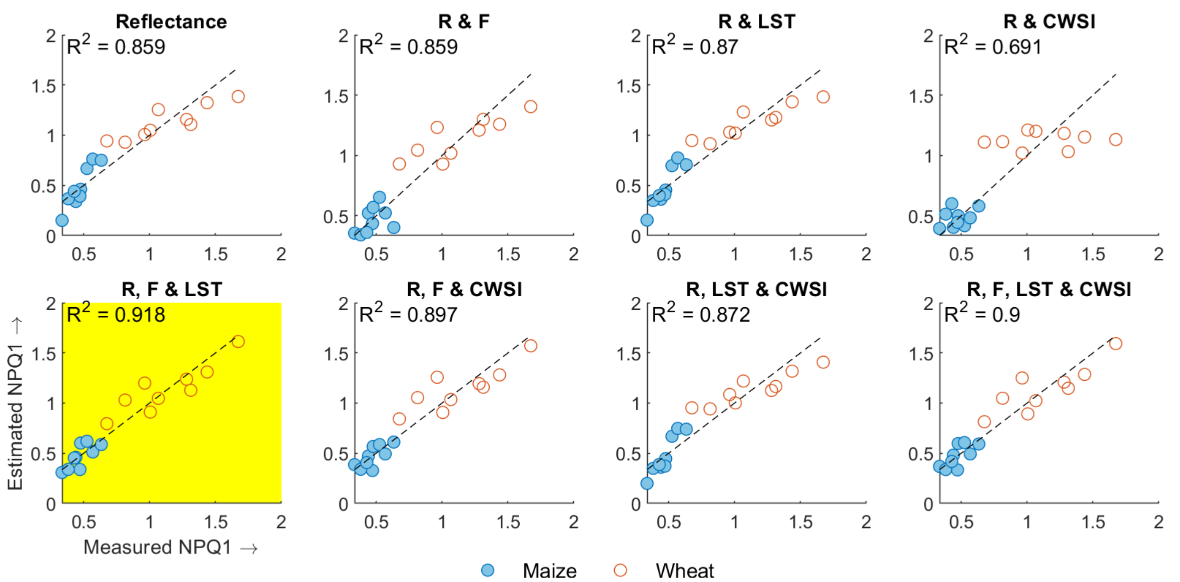


Figure 10: Mean squared error versus number of PLSR components to determine optimal number of components for each input combination for NPQ1 (upper part) and NPQ2 (lower part).



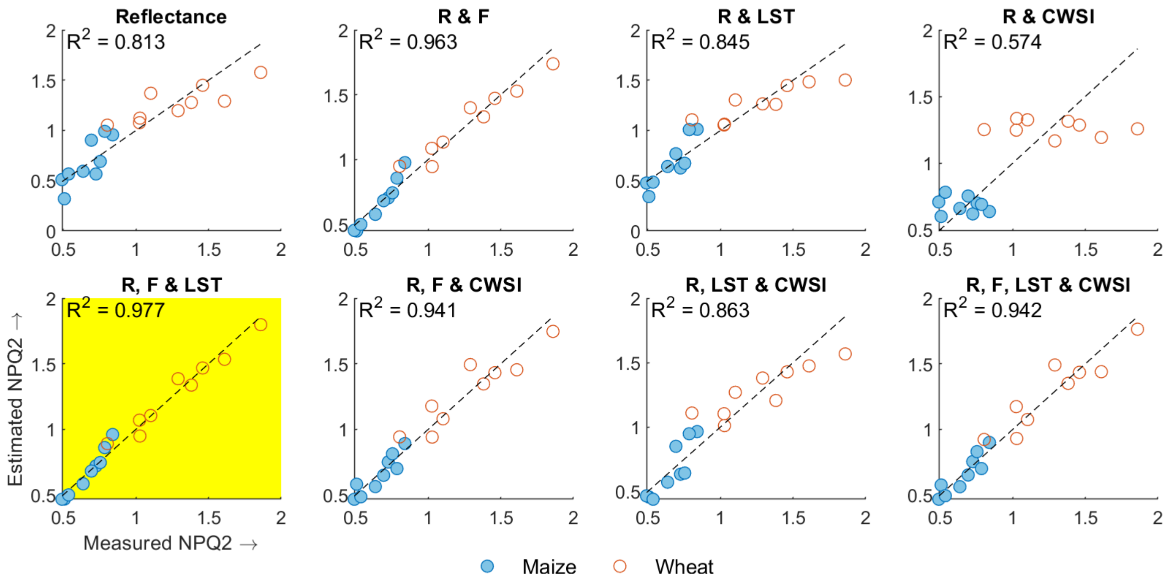


Figure 11: Scatterplots of measured versus estimated NPQ1 (upper part) and NPQ2 (lower part) for each input combination. The best variants are marked in yellow.

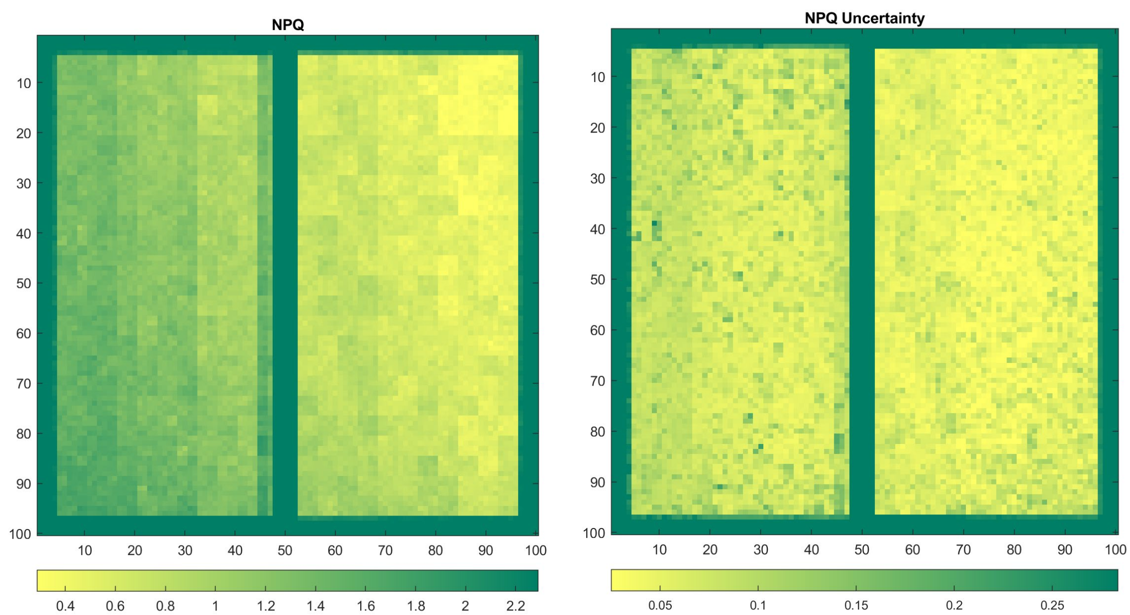


Figure 12: Resulting map and uncertainties.

#13

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

This document provides the participant with a structured template to report the methods used to estimate each of the biophysical or physiological variables required by the Spatial Scaling Challenge. After completing your analysis, fill out this form briefly and concisely.

Then copy/move the completed document to the folder /3_SCC_results/ without modifying its name and execute the last part of any of the scripts provided (SSC_script.py/m/R) to generate the compressed file to be sent to the Spatial Scaling Challenge organizers.

1. DISCUSSION

Vegetation status diagnosis

*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended)

There are significant variabilities of LAI, Cab, Vcmax,25, and NPQ in Fig. 1. These variabilities are due to plant functional types (C3/C4), plant nutrient stresses, and radiation intensity. In both maize and wheat plots, LAI, Cab, and Vcmax,25 variables have similar patterns. The higher LAI regions have higher Cab and Vcmax,25. This could be due to the fact that these three variables are closely linked with plant nutrient status and have very close relationships (Wang et al., 2021a, 2021b). The soil nutrient conditions possibly determine maize and wheat growth. Areas with less nutrient fertilization in soils tend to have lower LAI, Cab, and Vcmax,25.

However, NPQ is more complicated and related to photosynthetic energy partitioning among heat, photosynthetic reactions, and solar-induced fluorescence. NPQ2 (NPQ in noon times) of maize and wheat show different spatial patterns and values. Overall, wheat has higher NPQ values than maize, due to plant functional types. As a C3 plant, the light saturation for wheat is lower than the C4 plant maize. From meteorological records, we have high incoming radiation in these days and these high radiation leads to higher NPQ of Wheat than that of maize. Due to high radiation and air temperature, NPQ2 is higher than the morning NPQ (NPQ1). Furthermore, we also analyzed NPQ2-NPQ1, which shows the relative value changes within the day. We found that NPQ2-NPQ1 has a weak correlation with plant nutrient status (Cab). And possible other stress factors also contribute to the variabilities of NPQ.

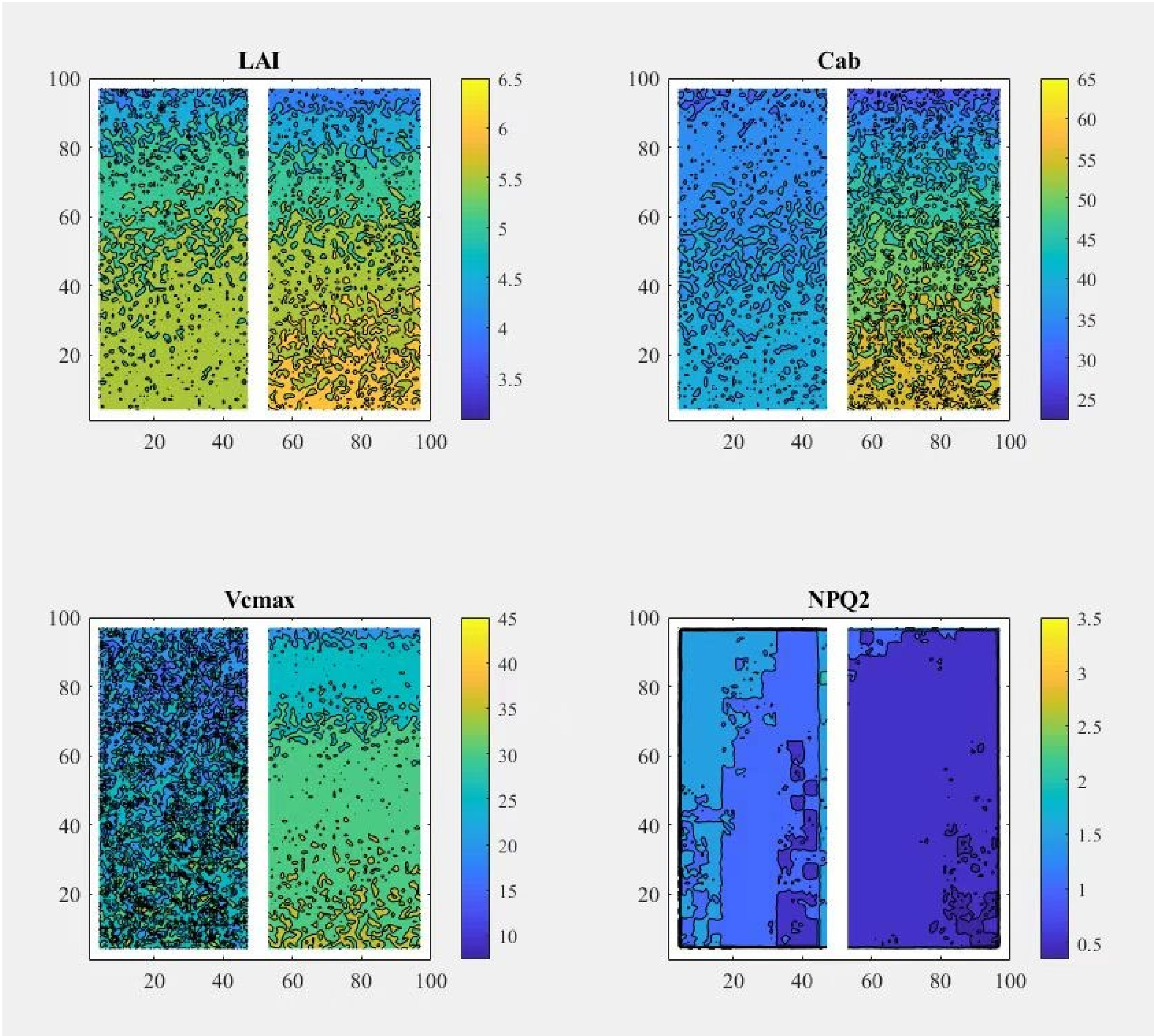


Fig. 1. Quantified leaf area index (LAI), chlorophyll content (Cab), photosynthetic capacity (Vcmax,25), and non-photochemical quenching (NPQ) from airborne hyperspectral, solar-induced fluorescence, and thermal infrared data. In each subplot, the left (west) figure is wheat *(Triticum aestivum) and the right (east) figure is maize (Zea mays).*

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

We used two approaches to quantify LAI. The first approach uses a single vegetation index (VI-based) and the empirical relationships between the VI and LAI. The second approach uses the SCOPE (mainly the radiative transfer modeling component, PROSAIL) model with machine learning surrogate modeling (RTM-based).
<u>*Which type of method do you use? (Remove those that do not apply)</u> 2: Empirical 3: Semi-empirical/Hybrid 4: Physically-based
<u>*Which are the input parameters or predictors of the algorithm?</u> *In the VI-based approach, NDVI is used to calculate wheat LAI, and Rededge is used for maize LAI.* *In the RTM-based approach, optical hyperspectral reflectance is the input to the model for predicting LAI.*
<u>*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)</u> *We used two approaches to quantify LAI. The first VI-based approach is empirical. We built the empirical linear relationships between several vegetation indices (VI, including NDVI, Rededge, and NIR_v) and in situ LAI. VIs were calculated from hyperspectral reflectance. We then compared the performance among these VIs and targeted the one with the largest R^2 and smallest RMSE. We found, in this case, NDVI ($(R_{780}-R_{660})/(R_{780}+R_{660})$) best simulated the wheat LAI (Eq. 1a) and Rededge (R_{750}/R_{705}) best for the maize LAI (Eq. 1b). We then applied these relationships to airborne hyperspectral imagery to predict LAI for every imagery pixel.* *Eq. 1a: LAI = 44.66*NDVI - 33.92 (wheat, adjusted R^2=0.79, RMSE=0.17)* *Eq. 1b: LAI = 1.09*Rededge + 0.40 (maize, adjusted R^2=0.77, RMSE=0.26)* *The second RTM-based approach is physically based and a hybrid of radiative transfer modeling and machine learning. We used SCOPE (PROSAIL) model simulations to generate synthetic datasets and then applied machine learning (random forest) to generate machine learning surrogate models to quantify LAI.* *Given that the VI-based approach is site-specific and the RTM-based approach can be generalized, we used the VI-based results and combined them with the plot measurements to validate the RTM-based results at both the plot and whole-field level. The comparison indicates that the LAI was underestimated by the RTM-based approach. RTM underestimation could be due to that PROSAIL simulating green LAI instead of total LAI.*

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])
<u>*Provide the name of the approach/method/algorithm used (add literature reference if applicable)</u> *We used two approaches to quantify Cab, similar to those used for LAI. The first one uses a single vegetation index (VI-based) and the second approach uses the SCOPE (PROSAIL) model with machine learning surrogate modeling (RTM-based, (Wang et al., 2021b Wang et al., 2021a).*
<u>*Which type of method do you use? (Remove those that do not apply)</u> 2: Empirical 4: Physically-based
<u>*Which are the input parameters or predictors of the algorithm?</u>

In the VI-based approach, Rededge is used to calculate Cab for both wheat and maize.

In the RTM-based approach, optical hyperspectral reflectance is input to the model for predicting Cab.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

We used two approaches to quantify Cab. The first approach is empirical. We built the empirical linear relationships between several vegetation indices (VI, including NDVI, Rededge, and NIR_v) and in situ Cab. VIs were calculated from hyperspectral reflectance. We then compared the performance among these VIs and targeted the one with the largest R2 and smallest RMSE. We found that Rededge (R750/R705) is the best VI to predict Cab for both wheat (Eq. 2a) and maize (Eq. 2b). We then applied these relationships to airborne hyperspectral imagery to predict Cab for every imagery pixel.

*Eq. 2a: Cab = 10.23*Rededge + 4.92 (wheat, adjusted R^2=0.86, RMSE=1.40)*

*Eq. 2b: Cab = 14.90*Rededge - 20.19 (maize, adjusted R^2=0.80, RMSE=3.26)*

The second approach uses SCOPE (PROSAIL) model simulations to generate synthetic datasets and then applies machine learning (random forest) to generate machine learning surrogate models to quantify Cab (Wang et al., 2021b) (Wang et al., 2021a). This approach is physically based and a hybrid of radiative transfer modeling and machine learning.

Given that the VI-based approach is site-specific and the RTM-based approach can be generalized, we used the VI-based results and combined them with the plot measurements to validate the RTM-based results at both the plot and whole-field level. The comparison indicated that overall, the two approaches had good agreements in the Cab estimation.

Leaf maximum carboxylation rate at 25 ºC ($V_{cmax,25}$, [μmol CO_2 cm^{-2} s^{-1}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

We used two approaches to quantify Vcmax,25. The first approach is VI-based empirical approach. The second approach is a hybrid one that first predicts Cab from RTM-based approach and then predicts Vcmax,25 from this predicted Cab and its statistical relationship developed with the field-measured Vcmax,25 (Wang et al., 2021a) (e.g. Wang et al., 2021b).

*Which type of method do you use? (Remove those that do not apply)

1: Statistical 2: Empirical 3: Semi-empirical/Hybrid

*Which are the input parameters or predictors of the algorithm?

Cab, one is calculated from the hyperspectral reflectance and the other is predicted by the RTM-based approach.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

From a mechanistic perspective, leaf maximum carboxylation rate could be most affected by leaf chlorophyll content (Cab). There are two ways to build an empirical relationship to predict Vcmax,25 – one is the relationship between Cab predicted by Rededge and Vcmax, 25, and the other is a direct relationship between Rededge and Vcmax, 25. In this study, we found that the direct Rededge-Vcmax,25 relationship performed better *than the predicted Cab-Vcmax,25 relationship. Therefore, Rededge was directly used to predict Vcmax,25 for both wheat (Eq. 3a) and maize (Eq. 3b).*

*Eq. 3a: Vcmax,25 = 25.78*Rededge – 62.85 (wheat, adjusted R^2=0.62, RMSE=6.76)*

*Eq. 3b: Vcmax,25 = 6.02*Rededge + 3.47 (maize, adjusted R^2=0.93, RMSE=0.76)*

The second approach, RTM-based hybrid, uses SCOPE (PROSAIL) model simulations to generate synthetic datasets and then applies machine learning (random forest) to generate machine learning surrogate models to quantify Cab (see the above Cab section,(Wang et al., 2021a) Wang et al., 2021b). This RTM-based Cab is then used to estimate Vcmax,25 by an empirical relationship as well.

Leaf non-photochemical quenching (*NPQ*, [-])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Energy-partitioning based empirical approach.

*Which type of method do you use? (Remove those that do not apply)

3: Semi-empirical/Hybrid

*Which are the input parameters or predictors of the algorithm?

SIF at 760 nm and Rededge index.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

The theoretical base of this empirical method is the energy partitioning among photosynthesis, SIF, and NPQ. We used the information in SIF and Rededge (R_{750}/R_{705}), which is a good proxy of chlorophyll content and we assumed to be a proxy of photosynthesis as well, to infer NPQ, i.e. the third component of the energy utilization. The linear regression with NPQ2 in field measurements suggested that SIF at 760 nm (SIF_{760}) and Rededge can explain 90% of the NPQ2 variations in the wheat field (Eq. 4a) and 70% in the maize field (Eq. 4b).

*Eq. 4a: NPQ2 = -1.58*SIF_{760} - 0.27*Rededge + 4.52 (wheat, adjusted R2=0.91, RMSE=0.10)*

*Eq. 4b: NPQ2 = -0.67*SIF_{760} – 0.15*Rededge + 2.83 (Maize, adjusted R2=0.70, RMSE=0.07)*

We also tested two additional VIs that are suggested in literature to be good proxies for NPQ, including PRI (Gamon et al., 1992) and NPQI (Peñuelas et al., 1995). Both VIs did not exhibit good relationships with NPQ in this study.

#14

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

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Then copy/move the completed document to the folder /3_SCC_results/ without modifying its name and execute the last part of any of the scripts provided (SSC_script.py/m/R) to generate the compressed file to be sent to the Spatial Scaling Challenge organizers.

1. DISCUSSION

Vegetation status diagnosis
*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended) *There are significant variabilities of LAI, Cab, Vcmax,25, and NPQ in Fig. 1. These variabilities are due to plant functional types (C3/C4), plant nutrient stresses, and radiation intensity. In both maize and wheat plots, LAI, Cab, and Vcmax,25 variables have similar patterns. The higher LAI regions have higher Cab and Vcmax,25. This could be due to the fact that these three variables are closely linked with plant nutrient status and have very close relationships (Wang et al., 2021a, 2021b). The soil nutrient conditions possibly determine maize and wheat growth. Areas with less nutrient fertilization in soils tend to have lower LAI, Cab, and Vcmax,25.* *However, NPQ is more complicated and related to photosynthetic energy partitioning among heat, photosynthetic reactions, and solar-induced fluorescence. NPQ2 (NPQ in noon times) of maize and wheat show different spatial patterns and values. Overall, wheat has higher NPQ values than maize, due to plant functional types. As a C3 plant, the light saturation for wheat is lower than the C4 plant maize. From meteorological records, we have high incoming radiation in these days and these high radiation leads to higher NPQ of Wheat than that of maize. Due to high radiation and air temperature, NPQ2 is higher than the morning NPQ (NPQ1). Furthermore, we also analyzed NPQ2-NPQ1, which shows the relative value changes within the day. We found that NPQ2-NPQ1 has a weak correlation with plant nutrient status (Cab). And possible other stress factors also contribute to the variabilities of NPQ.*

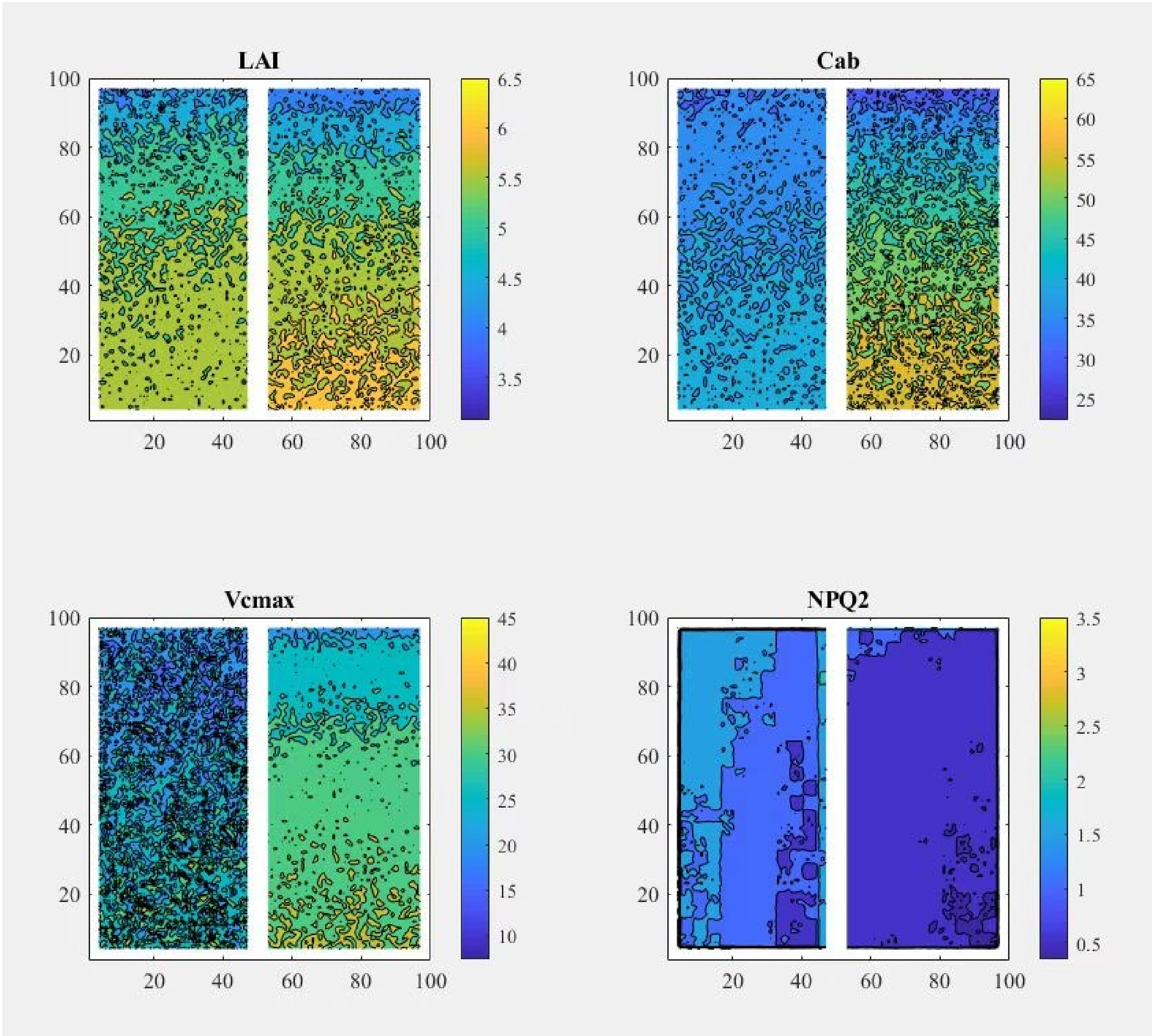


Fig. 1. Quantified leaf area index (LAI), chlorophyll content (Cab), photosynthetic capacity (Vcmax,25), and non-photochemical quenching (NPQ) from airborne hyperspectral, solar-induced fluorescence, and thermal infrared data. In each subplot, the left (west) figure is wheat (Triticum aestivum) and the right (east) figure is maize (Zea mays).

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

We used two approaches to quantify LAI. The first approach uses a single vegetation index (VI-based) and the empirical relationships between the VI and LAI. The second approach uses the SCOPE (mainly the radiative transfer modeling component, PROSAIL) model with machine learning surrogate modeling (RTM-based).

*Which type of method do you use? (Remove those that do not apply)

2: Empirical 3: Semi-empirical/Hybrid 4: Physically-based

*Which are the input parameters or predictors of the algorithm?

In the VI-based approach, NDVI is used to calculate wheat LAI, and Rededge is used for maize LAI.

In the RTM-based approach, optical hyperspectral reflectance is the input to the model for predicting LAI.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

We used two approaches to quantify LAI. The first VI-based approach is empirical. We built the empirical linear relationships between several vegetation indices (VI, including NDVI, Rededge, and NIR_v) and in situ LAI. VIs were calculated from hyperspectral reflectance. We then compared the performance among these VIs and targeted the one with the largest R^2 and smallest RMSE. We found, in this case, NDVI ($(R_{780}-R_{660})/(R_{780}+R_{660})$) best simulated the wheat LAI (Eq. 1a) and Rededge (R_{750}/R_{705}) best for the maize LAI (Eq. 1b). We then applied these relationships to airborne hyperspectral imagery to predict LAI for every imagery pixel.

*Eq. 1a: LAI = 44.66*NDVI - 33.92 (wheat, adjusted R^2=0.79, RMSE=0.17)*

*Eq. 1b: LAI = 1.09*Rededge + 0.40 (maize, adjusted R^2=0.77, RMSE=0.26)*

The second RTM-based approach is physically based and a hybrid of radiative transfer modeling and machine learning. We used SCOPE (PROSAIL) model simulations to generate synthetic datasets and then applied machine learning (random forest) to generate machine learning surrogate models to quantify LAI.

Given that the VI-based approach is site-specific and the RTM-based approach can be generalized, we used the VI-based results and combined them with the plot measurements to validate the RTM-based results at both the plot and whole-field level. The comparison indicates that the LAI was underestimated by the RTM-based approach. RTM underestimation could be due to that PROSAIL simulating green LAI instead of total LAI.

Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

We used two approaches to quantify Cab, similar to those used for LAI. The first one uses a single vegetation index (VI-based) and the second approach uses the SCOPE (PROSAIL) model with machine learning surrogate modeling (RTM-based, (Wang et al., 2021b) Wang et al., 2021a).

*Which type of method do you use? (Remove those that do not apply)

2: Empirical 4: Physically-based

*Which are the input parameters or predictors of the algorithm?

In the VI-based approach, Rededge is used to calculate Cab for both wheat and maize.

In the RTM-based approach, optical hyperspectral reflectance is input to the model for predicting Cab.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

We used two approaches to quantify Cab. The first approach is empirical. We built the empirical linear relationships between several vegetation indices (VI, including NDVI, Rededge, and NIR_v) and in situ Cab. VIs were calculated from hyperspectral reflectance. We then compared the performance among these VIs and targeted the one with the largest R2 and smallest RMSE. We found that Rededge (R750/R705) is the best VI to predict Cab for both wheat (Eq. 2a) and maize (Eq. 2b). We then applied these relationships to airborne hyperspectral imagery to predict Cab for every imagery pixel.

*Eq. 2a: Cab = 10.23*Rededge + 4.92 (wheat, adjusted R^2=0.86, RMSE=1.40)*

*Eq. 2b: Cab = 14.90*Rededge - 20.19 (maize, adjusted R^2=0.80, RMSE=3.26)*

The second approach uses SCOPE (PROSAIL) model simulations to generate synthetic datasets and then applies machine learning (random forest) to generate machine learning surrogate models to quantify Cab (Wang et al., 2021b) (Wang et al., 2021a). This approach is physically based and a hybrid of radiative transfer modeling and machine learning.

Given that the VI-based approach is site-specific and the RTM-based approach can be generalized, we used the VI-based results and combined with the plot measurements to validate the RTM-based results at both the plot and whole-field level. The comparison indicated that overall, the two approaches had good agreements in the Cab estimation.

Leaf maximum carboxylation rate at 25 °C ($V_{cmax,25}$, [μmol CO_2 cm^{-2} s^{-1}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

We used two approaches to quantify Vcmax,25. The first approach is VI-based empirical approach. The second approach is a hybrid one that first predicts Cab from RTM-based approach and then predicts Vcmax,25 from this predicted Cab and its statistical relationship developed with the field-measured Vcmax,25 (Wang et al., 2021a) (e.g. Wang et al., 2021b).

*Which type of method do you use? (Remove those that do not apply)

1: Statistical 2: Empirical 3: Semi-empirical/Hybrid

*Which are the input parameters or predictors of the algorithm?

Cab, one is calculated from the hyperspectral reflectance and the other is predicted by the RTM-based approach.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

From a mechanistic perspective, leaf maximum carboxylation rate could be most affected by leaf chlorophyll content (Cab). There are two ways to build an empirical relationship to predict Vcmax,25 – one is the relationship between Cab predicted by Rededge and Vcmax, 25, and the other is a direct relationship between Rededge and Vcmax, 25. In this study, we found that the direct Rededge-Vcmax,25 relationship performed better than the predicted Cab-Vcmax,25 relationship. Therefore, Rededge was directly used to predict Vcmax,25 for both wheat (Eq. 3a) and maize (Eq. 3b).

*Eq. 3a: Vcmax,25 = 25.78*Rededge – 62.85 (wheat, adjusted R^2=0.62, RMSE=6.76)*

*Eq. 3b: Vcmax,25 = 6.02*Rededge + 3.47 (maize, adjusted R^2=0.93, RMSE=0.76)*

The second approach, RTM-based hybrid, uses SCOPE (PROSAIL) model simulations to generate synthetic datasets and then applies machine learning (random forest) to generate machine learning surrogate models to quantify Cab (see the above Cab section, (Wang et al., 2021a) Wang et al., 2021b). This RTM-based Cab is then used to estimate Vcmax,25 by an empirical relationship as well.

Leaf non-photochemical quenching (*NPQ*, [-])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Energy-partitioning based empirical approach.

*Which type of method do you use? (Remove those that do not apply)

3: Semi-empirical/Hybrid

*Which are the input parameters or predictors of the algorithm?

SIF at 760 nm and Rededge index.

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

The theoretical base of this empirical method is the energy partitioning among photosynthesis, SIF, and NPQ. We used the information in SIF and Rededge (R_{750}/R_{705}), which is a good proxy of chlorophyll content and we assumed to be a proxy of photosynthesis as well, to infer NPQ, i.e. the third component of the energy utilization. The linear regression with NPQ2 in field measurements suggested that SIF at 760 nm (SIF_{760}) and Rededge can explain 90% of the NPQ2 variations in the wheat field (Eq. 4a) and 70% in the maize field (Eq. 4b).

Eq. 4a: $NPQ2 = -1.58*SIF_{760} - 0.27*Rededge + 4.52$ (wheat, adjusted R2=0.91, RMSE=0.10)

Eq. 4b: $NPQ2 = -0.67*SIF_{760} – 0.15*Rededge + 2.83$ (Maize, adjusted R2=0.70, RMSE=0.07)

We also tested two additional VIs that are suggested in literature to be good proxies for NPQ, including PRI (Gamon et al., 1992) and NPQI (Peñuelas et al., 1995). Both VIs did not exhibit good relationships with NPQ in this study.

#15

SPATIAL SCALING CHALLENGE
DESCRIPTION OF THE METHODS

This document provides the participant with a structured template to report the methods used to estimate each of the biophysical or physiological variables required by the Spatial Scaling Challenge. After completing your analysis, fill out this form briefly and concisely.

Then copy/move the completed document to the folder /3_SCC_results/ without modifying its name and execute the last part of any of the scripts provided (SSC_script.py/m/R) to generate the compressed file to be sent to the Spatial Scaling Challenge organizers.

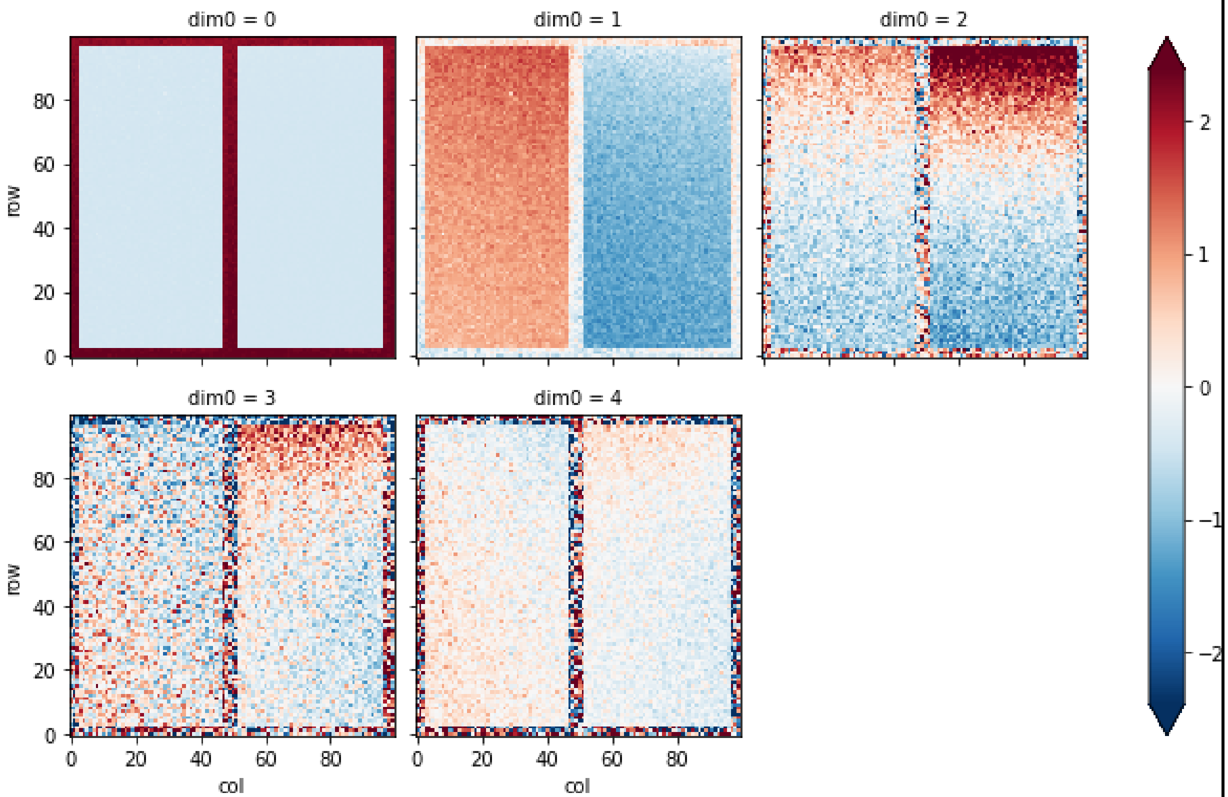
1. DISCUSSION

Vegetation status diagnosis
*From the data analyzed, what can you conclude about the observed vegetation's health/stress/physiological status? (max. 250 words recommended) *Answer here*

2. METHODS

Leaf area index (*LAI*, [m^2 m^{-2}])
*Provide the name of the approach/method/algorithm used (add literature reference if applicable) Gaussian Process Regression using the field measurements as training points
*Which type of method do you use? (Remove those that do not apply) 1: Statistical 2: Empirical
*Which are the input parameters or predictors of the algorithm? Aerial HSI
*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable) Prior to dimensionality reduction, data were filtered with a median filter (window size=3) in the spectral domain only. Input dimensionality was reduced to 5D using principal component analysis, explaining 99.9% of the variance in the dataset. 99.7% of the variance was explained by the first principal component that differentiated the crop area from the field margin and only 0.02% of the variance remained in the subsequent PCs (explaining

the within-field variance). The 5D representation of the spectrum was used as the input to a Gaussian Process Regressor (GPR). The response variable (LAI) was zero-centred to remove the need to fit an offset. A compound Matern (5/2) and White Noise kernel was fit using the Laplace Approximation (default Scikit-Learn).



Leaf chlorophyll content (C_{ab}, [µg cm^{-2}])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Gaussian Process Regression using the field measurements as training points

*Which type of method do you use? (Remove those that do not apply)

1: Statistical 2: Empirical

*Which are the input parameters or predictors of the algorithm?

Aerial HSI

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

As for LAI

Leaf maximum carboxylation rate at 25 °C ($V_{cmax,25}$, [$\mu mol\ CO_2\ cm^{-2}\ s^{-1}$])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Gaussian Process Regression using the field measurements as training points

*Which type of method do you use? (Remove those that do not apply)

1: Statistical 2: Empirical

*Which are the input parameters or predictors of the algorithm?

Aerial HSI

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

As for LAI

Leaf non-photochemical quenching (*NPQ*, [-])

*Provide the name of the approach/method/algorithm used (add literature reference if applicable)

Gaussian Process Regression using the field measurements as training points

*Which type of method do you use? (Remove those that do not apply)

1: Statistical 2: Empirical

*Which are the input parameters or predictors of the algorithm?

LAI (determined above), Fluorescence imagery

*Briefly and concisely describe the method you used to predict this variable (and uncertainties if you did) with a formal style. This section might be included in the joint manuscript (max. 250 words recommended; add literature reference if applicable)

LAI and the two fluorescent radiance values were used as the input to predict NPQ using a Gaussian Process Regressor (GPR). The response variable (LAI) was zero-centred to remove the need to fit an offset. A compound Matern (5/2) and White Noise kernel was fit using the Laplace Approximation (default Scikit-Learn).

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Table S1.1. Spatial Scaling Challenge questionnaire

Contributor	How did you combined remote sensing imagery of different spatial resolutions and field data?	How did you used field NPQ data?	If you used a statistical/hybrid inversion approach, how did you estimate LAI, Cab, Vcmax,25 and NPQ?	If you worked with the SCOPE model, which version you run?	If you worked with the SCOPE model, which sub-modules you used? (multiple answers allowed)
#01	I used the data at the original spatial resolutino of each sensor	I used only one of the rounds of NPQ measurements (NPQ2)	Each variable was predicted from a different model	I did not use SCOPE	
#02	I used the data at the original spatial resolutino of each sensor	I used only one of the rounds of NPQ measurements (NPQ1)	Each variable was predicted from a different model	I did not use SCOPE	
#03	We smoothed across several resolutions in a spatial series, but basically the second.	We didn't use field NPQ, SCOPE-estimated NPQ was accepted based on the most accurate fluorescence output by SCOPE.	Two variables were predicted from the same model	SCOPE v2.x	RTMf (RTM for fluorescence fluxes), RTMz (RTM for fluxes induced by the xanthophyll cycle), biochemical (biochemical model for photosystem energy partitioning)
#04	I used the data at the original spatial resolutino of each sensor	I used only one of the rounds of NPQ measurements (NPQ2)	Each variable was predicted from a different model	SCOPE v2.x	
#05	I used the data at the original spatial	I used only one of the rounds of NPQ	Each variable was predicted from a	I did not use SCOPE	

	resolutino of each sensor	measurements (NPQ2)	different model		
#06	I used the data at the original spatial resolutino of each sensor	I used only one of the rounds of NPQ measurements (NPQ1)	Each variable was predicted from a different model	I did not use SCOPE	
#07	I used the data at the original spatial resolutino of each sensor	I used both rounds of NPQ measurements (NPQ1 and NPQ2)	Each variable was predicted from a different model	SCOPE v2.x	BSM (simulating soil reflectance), RTMf (RTM for fluorescence fluxes), biochemical (biochemical model for photosystem energy partitioning)
#08	I used the data at the original spatial resolutino of each sensor	I used only one of the rounds of NPQ measurements (NPQ1)	Each variable was predicted from a different model	I did not use SCOPE	
#09	I used the data at the original spatial resolutino of each sensor	I used only one of the rounds of NPQ measurements (NPQ1)	Each variable was predicted from a different model	I did not use SCOPE	
#10	I used the data at the original spatial resolutino of each sensor	I used only one of the rounds of NPQ measurements (NPQ1)	Each variable was predicted from a different model	I did not use SCOPE	
#11	I used the data at the original spatial resolution of ONE sensor (HDRF)	I used NPQ to understand how to average sunlit and shaded leaves to match the range		SCOPE v2.x	BSM (simulating soil reflectance), RTMo (RTM for incident-reflected radiation), biochemical (biochemical model for

					photosystem energy partitioning), ebal (energy balance module)
#12	I used the data at the original spatial resolutino of each sensor	I used both rounds of NPQ measurements (NPQ1 and NPQ2)	Each variable was predicted from a different model	I did not use SCOPE	
#13	I down-graded to the coarsest resolution	I used only one of the rounds of NPQ measurements (NPQ2)	Two variables were predicted from the same model	SCOPE v2.x	BSM (simulating soil reflectance), RTMo (RTM for incident-reflected radiation), RTMz (RTM for fluxes induced by the xanthophyll cycle)
#14	I down-graded to the coarsest resolution	I used only one of the rounds of NPQ measurements (NPQ2)	Two variables were predicted from the same model	SCOPE v2.x	BSM (simulating soil reflectance), RTMo (RTM for incident-reflected radiation), RTMz (RTM for fluxes induced by the xanthophyll cycle)
#15	I used the data at the original spatial resolutino of each sensor	I used only one of the rounds of NPQ measurements (NPQ1)	Each variable was predicted from a different model	I did not use SCOPE	